

Monitoring derivation of the quantum linear Boltzmann equation

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We show how the effective equation of motion for a distinguished quantum particle in an ideal gas environment can be obtained by means of the monitoring approach introduced in [EPL 77, 50007 (2007)]. The resulting Lindblad master equation accounts for the quantum effects of the scattering dynamics in a non-perturbative fashion and it describes decoherence and dissipation in a unified framework. It incorporates various established equations as limiting cases and reduces to the classical linear Boltzmann equation once the state is diagonal in momentum.

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I. INTRODUCTION

A basic problem in the field of open quantum dynamics is the question how the motion of a tracer particle, such as a Brownian particle, is affected by the presence of a background gas [1]. More specifically, one may consider a single distinguished test particle which moves in the absence of external forces, but is interacting with an ideal, non-degenerate, and stationary gas. The elastic collisions with the gas particles will affect the motional state of the tracer particle, and we are interested in the appropriate effective equation of motion for its (reduced) density operator which incorporates the interaction process in a non-perturbative manner. This master equation is necessarily linear, since it pertains to a single particle, and it is aptly called, in analogy to the case of a classical tracer particle [2], the *quantum linear Boltzmann equation* (QLBE). However, one should not confuse it with a *linearized* quantum equation for the single particle gas state of a self-interacting quantum gas, sometimes called by the same name (though the notation “linearized quantum Boltzmann equation” would seem more fitting).

The dynamics to be described by the QLBE can be quite involved because the tracer particle may be in a very non-trivial motional state, characterized for example by the non-classical correlations between different position and momentum components found in a matter wave interferometer [3]. On the long run, the tracer particle will approach a stationary “thermalized” state, while the ever increasing entanglement with the gas will reduce its quantum coherences already on much shorter time scales. A limiting case occurs if the tracer particle can be taken as infinitely massive, so that energy exchange during the collisions can be safely neglected. In this case one expects pure collisional decoherence, i.e., a spatial “localization” of an extended coherent matter wave into a mixture with

reduced spatial coherence.

This problem was first investigated by Joos and Zeh in a linearized description [4]. However, a *non-perturbative* treatment is required to describe how the spatial coherences in an interfering state get reduced the more the better the scattered gas particles can “resolve” the different interference paths, and to account for the saturation of this effect with increasing path difference [5, 6]. This loss of coherence, which may be related to the “which path” information revealed to the environment, was observed experimentally with interfering fullerene molecules in good quantitative agreement with decoherence theory [7].

The situation is much more involved if the ratio m/M between the mass m of the gas particles and the mass M of the tracer particle cannot be neglected. In this case the particle experiences friction, it will dissipate its energy and finally thermalize. The appropriate effective equation must then be able to describe the full interplay of decohering and dissipative dynamics. An important advancement in this direction was the proposal by Diósi [8] of an equation based on a combination of scattering theory and heuristic arguments. In this derivation a number of ad-hoc approximations had to be introduced when incorporating the Markov assumption in order to end up with a time-local master equation in Lindblad form. As is notorious in non-perturbative derivations of Markovian master equations, these approximations are not unambiguous and very hard to motivate microscopically.

One way to overcome this ambiguity problem was recently proposed by one of us [9]. This method, called the monitoring approach, treats the Markov assumption not as an approximation to be performed when tracing out the environmental degrees of freedom, but incorporates it before this trace is done by combining concepts from the theory of generalized and continuous measurements with time dependent scattering theory. When applied to the present case, the essential premise of this approach is to assume that both the rate and the effect of indi-

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vidual collisions between the tracer and the gas particles are separately well defined. The Markov assumption then enters by saying that three-particle collisions are sufficiently unlikely to be safely neglected, as are subsequent collisions with the same gas molecule within the relevant time scale. This assumption excludes liquefied or strongly self-interacting “gas” environments, but it seems natural in the case of an ideal gas in a stationary state. The only real freedom in this framework of the monitoring approach lies in the choice of two microscopic operators. Selecting the operators suggested by microscopic scattering theory then leads to the equation in an unambiguous way.

The present result was already announced in [10]. Here we give a more detailed derivation¹, presenting two independent ways of evaluating the environmental trace. We will also point out that various limits reduce the QLBE to well-established results. In particular, one obtains the weak-coupling version of the QLBE, proposed earlier by one of us [11, 12, 13], if the appropriate limit is taken by replacing the scattering amplitudes with their Born approximation. Other limits lead to the generalized form of the Caldeira-Leggett master equation [14], the master equation of pure collisional decoherence, and the classical linear Boltzmann equation.

The structure of the article is as follows. In Sect. II we briefly review the monitoring approach and specify the microscopic operators for the problem at hand. Before delving into the calculations we present the form of the resulting QLBE in momentum representation in Sect. III. This allows us to discuss the relation of the QLBE to the classical linear Boltzmann equation. Section IV then starts out with the calculation in momentum basis and explains why a straightforward evaluation of the trace is impossible. A first remedy, based on the restriction to wave packet states of incoming type is given in Sect. V. Section VI provides an alternative way of doing the environmental trace, which is based on a formal redefinition of the scattering operator. Section VII is devoted to calculating the coherent modification part of the master equation using the same wave packet technique as in Sect. V. The basis independent “operator form” of the QLBE is obtained in Sect. VIII; it shows immediately that the master equation provides the generator of a completely positive and translationally invariant quantum dynamical semigroup. Section IX summarizes the various limiting forms of the QLBE, and we present our conclusions in Sect. X.

¹ We emphasize that the word “derivation” is used here in the physicist’s sense, implying that arguments and approximations are invoked which—though physically stringent and leading to a uniquely distinguished equation—may be hard to substantiate in a proper mathematical framework. We certainly do not claim to provide a mathematically rigorous proof, noting that even the classical Boltzmann equation still lacks such a mathematical derivation.

II. THE MONITORING MASTER EQUATION FOR A TRACER PARTICLE IN A GAS

A. The monitoring master equation

Let us start with a brief review of the monitoring approach [9]. It yields a Markovian master equation that is specified, apart from the system Hamiltonian H , in terms of two operators, a *rate operator* Γ and a *scattering operator* S .

The operator Γ is *positive* and in the present context it has the defining property that its expectation value yields the probability of collision with the gas particles in the small time interval Δt ,

$$\Pr(C_{\Delta t}|\rho \otimes \rho_{\text{gas}}) = \text{Tr}(\Gamma[\rho \otimes \rho_{\text{gas}}])\Delta t + \mathcal{O}(\Delta t^2) \quad (1)$$

Here, ρ is the system density operator which describes, in the present application, the motional state of the tracer particle. The operator ρ_{gas} is the effective single particle state of the gas environment, and it is assumed to be stationary (but not necessarily in thermal equilibrium). Thus, Γ acts in a two-particle Hilbert space, and its task is to incorporate the tracer state-dependence of the collision probability into the dynamic formulation.

The scattering operator S , on the other hand, is *unitary*, and by definition it yields the two particle state after a single collision, so that, upon tracing over the gas particle, we obtain the new tracer particle state (in interaction picture) after a single scattering event took place [15],

$$\rho' = \text{Tr}_{\text{gas}}(S[\rho \otimes \rho_{\text{gas}}]S^\dagger). \quad (2)$$

The monitoring approach [9] now implements the Markov assumption by combining the state dependence of the collision probability (1) with the transformation (2) in a way which is consistent with the state transformation rules of quantum mechanics [16], using concepts of the theory of generalized and continuous measurements [17, 18, 19]. In the Schrödinger picture one thus obtains the effective equation of motion

$$\frac{d}{dt}\rho = \frac{1}{i\hbar}[H, \rho] + \mathcal{L}\rho + \mathcal{R}\rho. \quad (3)$$

The superoperators \mathcal{L} and \mathcal{R} are best specified in terms of the nontrivial part T of the scattering operator $S = I + iT$. The part $\mathcal{L}\rho$ then takes the form [9]

$$\begin{aligned} \mathcal{L}\rho = & \text{Tr}_{\text{gas}}\left(T\Gamma^{1/2}[\rho \otimes \rho_{\text{gas}}]\Gamma^{1/2}T^\dagger\right) \\ & - \frac{1}{2}\text{Tr}_{\text{gas}}\left(\Gamma^{1/2}T^\dagger T\Gamma^{1/2}[\rho \otimes \rho_{\text{gas}}]\right) \\ & - \frac{1}{2}\text{Tr}_{\text{gas}}\left([\rho \otimes \rho_{\text{gas}}]\Gamma^{1/2}T^\dagger T\Gamma^{1/2}\right). \end{aligned} \quad (4)$$

It describes the incoherent evolution of ρ due to the presence of the gas environment. The part $\mathcal{R}\rho$, on the other

hand, is given by²

$$\mathcal{R}\rho = i \text{Tr}_{\text{gas}} \left(\left[\Gamma^{1/2} \text{Re}(\mathbf{T}) \Gamma^{1/2}, \rho \otimes \rho_{\text{gas}} \right] \right), \quad (5)$$

where $\text{Re}(\mathbf{T}) = (\mathbf{T} + \mathbf{T}^\dagger)/2$. It is responsible for a unitary modification of the evolution, a renormalization of the system energy due to the coupling with the environment.

We would like to emphasize that the evolution described by (3) is non-perturbative in the sense that the collisional transformation described by \mathbf{S} is not assumed to be weak. Moreover, note that the incoherent part (4) is manifestly Markovian even before the environmental trace is done.

B. Rate and scattering operators

In the framework of the monitoring approach the only essential freedom lies in the choice of the operators Γ , \mathbf{T} , and \mathbf{H} appearing in Eqs. (3)-(5). In this section we will specify them on a microscopic basis. Before that it is helpful to consider with some care ρ_{gas} , the effective single particle state of an ideal gas with number density n_{gas} .

To be describable by a normalizable state, the gas must be confined, say with periodic boundary conditions, to a finite spatial region Ω with (large) normalization volume $|\Omega|$. Let us denote the projector to this spatial region as

$$\mathbf{l}_\Omega = \int_\Omega d\mathbf{x} |\mathbf{x}\rangle\langle\mathbf{x}|. \quad (6)$$

Using the double-bracket notation $||\mathbf{p}\rangle\rangle$ for the volume-normalized momentum states, the density operators corresponding to these proper vectors take the form

$$\rho_{\mathbf{p}} = ||\mathbf{p}\rangle\rangle\langle\langle\mathbf{p}| = \frac{(2\pi\hbar)^3}{|\Omega|} \mathbf{l}_\Omega |\mathbf{p}\rangle\langle\mathbf{p}| \mathbf{l}_\Omega. \quad (7)$$

Here the $|\mathbf{p}\rangle$ are the usual improper momentum eigenvectors, $\langle\mathbf{x}|\mathbf{p}\rangle = (2\pi\hbar)^{-3/2} \exp(i\mathbf{x} \cdot \mathbf{p}/\hbar)$. Since ρ_{gas} is stationary it must be a convex combination of the pure momentum states (7). It is completely characterized by the gas momentum distribution $\mu(\mathbf{p})$, a positive function satisfying $\int d\mathbf{p} \mu(\mathbf{p}) = 1$. Thus ρ_{gas} has the form

$$\rho_{\text{gas}} = \int d\mathbf{p} \mu(\mathbf{p}) \rho_{\mathbf{p}} = \frac{(2\pi\hbar)^3}{|\Omega|} \mathbf{l}_\Omega \mu(\mathbf{p}) \mathbf{l}_\Omega, \quad (8)$$

where \mathbf{p} is the unrestricted momentum operator of a single gas particle. This state is normalized, $\text{Tr}(\rho_{\text{gas}}) = 1$, and it is uniform in position, $\langle\mathbf{x}|\rho_{\text{gas}}|\mathbf{x}\rangle = 1/|\Omega|$ for

$\mathbf{x} \in \Omega$. The most natural choice for μ is of course the Maxwell-Boltzmann distribution, see (94) below, but we will keep μ unspecified in order to indicate that the particular form of μ is not relevant for most of what follows.

In principle, projections similar to the \mathbf{l}_Ω in (8) are also needed when defining the operators Γ , \mathbf{T} , and \mathbf{H} of (3)-(5). To avoid clumsy notation we will instead present them in their unrestricted form and take care of the restrictions during the calculations below.

Since the tracer particle is supposed to move in the absence of external forces the Hamiltonian part of (3) is given by $\mathbf{H} = \mathbf{P}^2/2M$, where \mathbf{P} is the momentum operator of the tracer particle. The two-particle operators Γ and \mathbf{T} depend on the relative coordinates between tracer and gas particle, and it will be convenient to denote relative momenta by

$$\text{rel}(\mathbf{p}, \mathbf{P}) := \frac{m_*}{m} \mathbf{p} - \frac{m_*}{M} \mathbf{P} \quad (9)$$

with $m_* = mM/(M+m)$ the reduced mass. Thus, the momentum dyadics corresponding to the different factorizations of the total Hilbert space $\mathcal{H}_{\text{tot}} = \mathcal{H} \otimes \mathcal{H}_{\text{gas}} = \mathcal{H}_{\text{cm}} \otimes \mathcal{H}_{\text{rel}}$ are related by

$$|\mathbf{P}\rangle\langle\mathbf{P}'| \otimes |\mathbf{p}\rangle\langle\mathbf{p}'|_{\text{gas}} = |\mathbf{P} + \mathbf{p}\rangle\langle\mathbf{P}' + \mathbf{p}'|_{\text{cm}} \otimes |\text{rel}(\mathbf{p}, \mathbf{P})\rangle\langle\text{rel}(\mathbf{p}', \mathbf{P}')|_{\text{rel}}. \quad (10)$$

In classical mechanics, the collision rate is obtained by multiplying the current density $j_0(\mathbf{p}, \mathbf{P}) = n_{\text{gas}} |\text{rel}(\mathbf{p}, \mathbf{P})|/m_*$ of the relative motion with the total scattering cross section σ_{tot} (which also depends on the relative momentum). It seems therefore natural to define Γ as the corresponding operator on $\mathcal{H}_{\text{cm}} \otimes \mathcal{H}_{\text{rel}}$,

$$\begin{aligned} \Gamma &= \mathbf{l}_{\text{cm}} \otimes [j_0(\mathbf{p}, \mathbf{P}) \sigma_{\text{tot}}(\text{rel}(\mathbf{p}, \mathbf{P}))]_{\text{rel}} \\ &= \mathbf{l}_{\text{cm}} \otimes [\Gamma_0]_{\text{rel}} \end{aligned} \quad (11)$$

with

$$\Gamma_0 = \frac{n_{\text{gas}}}{m_*} |\text{rel}(\mathbf{p}, \mathbf{P})| \sigma_{\text{tot}}(\text{rel}(\mathbf{p}, \mathbf{P})). \quad (12)$$

Indeed, for normalized and separable particle-gas states the expectation value of this operator yields the collision rate experienced by the tracer particle, provided their relative state is of *incoming type*. If the two-particle state is of outgoing type, on the other hand, the motion of the relative coordinate is directed away from the origin, so that the particle and the gas molecule never interact. Still, the operator (11) would yield a finite expectation value in that case, since it depends only on the modulus of the relative velocity and not its orientation. A proper definition of Γ should therefore also include a projection to the subspace of truly incoming relative motional states. Unfortunately, it is rather difficult to formulate this projection in a way so that one can work with it in concrete calculations. Therefore, instead of using a more refined definition we shall stick with Eq. (11) keeping in mind that it is valid only for incoming states of the relative motion.

² A marginally different expression was given in Ref. [9], see the discussion in Sect. VII.

As the last step, we have to define the operator $S = I + iT$ describing the effect of a single collision. It is natural to use scattering theory for a microscopic definition [15]. The center-of-mass coordinate then remains unaffected,

$$S = I_{\text{cm}} \otimes [S_0]_{\text{rel}} \quad (13)$$

and the scattering operator of the relative coordinates $S_0 = I + iT_0$ is fully specified in terms of the complex scattering amplitudes $f(\mathbf{p}_f, \mathbf{p}_i)$, which are determined by the inter-particle potential [20],

$$\langle \mathbf{p}_f | T_0 | \mathbf{p}_i \rangle = \frac{1}{2\pi\hbar} \delta\left(\frac{p_f^2 - p_i^2}{2}\right) f(\mathbf{p}_f, \mathbf{p}_i). \quad (14)$$

Note that a delta-function in (14) ensures that the energy is conserved during an elastic collision changing the relative momentum from \mathbf{p}_i to \mathbf{p}_f .

The scattering amplitude also defines the cross section required in (11). The differential cross section is given by

$$\sigma(\mathbf{p}_f, \mathbf{p}_i) = |f(\mathbf{p}_f, \mathbf{p}_i)|^2 \quad (15)$$

and the total cross section reads

$$\sigma_{\text{tot}}(\mathbf{p}_i) = \int d\mathbf{n} |f(\mathbf{p}_i \mathbf{n}, \mathbf{p}_i)|^2, \quad (16)$$

where \mathbf{n} is a unit vector with $d\mathbf{n}$ the associated solid angle element.

It is important to keep in mind that the S-matrix (13) provided by scattering theory is physically meaningful only for proper incoming states of the relative motion, even though it is defined on the whole Hilbert space. This is schematically shown in Fig. 1 where we contrast the action of S_0 on an incoming wave packet with its effect on an outgoing state, showing that an outgoing wave packet may get spuriously transformed. The reason is that the Møller operator $\hat{\Omega}_+ = \lim_{t \rightarrow \infty} U(t) U_0(-t)$ used to construct $S_0 = \hat{\Omega}_+^\dagger \hat{\Omega}_+$ involves a free *backward* evolution in time $U_0(-t)$, followed by a forward motion $U(t)$ in the presence of the interaction potential. To avoid this undesired transformation in (3) we must either ensure that outgoing wave packets contribute with a zero collision rate or we have to modify S_0 such that it leaves the outgoing contributions invariant.

III. THE QLBE IN MOMENTUM REPRESENTATION

Before we proceed to derive the quantum linear Boltzmann equation let us present the result in the basis of improper momentum eigenstates $|\mathbf{P}\rangle$, where it takes a particularly simple form. This permits to introduce the complex rate function M_{in} to be evaluated in Sects. IV–VI, and to discuss its relation to the classical rate densities of the collision kernel.

We will see that the momentum representation of the incoherent part (4) of the QLBE can be written in terms of a single complex function, and that it takes the form

$$\begin{aligned} \langle \mathbf{P} | \mathcal{L} \rho | \mathbf{P}' \rangle &= \int d\mathbf{Q} \langle \mathbf{P} - \mathbf{Q} | \rho | \mathbf{P}' - \mathbf{Q} \rangle M_{\text{in}}(\mathbf{P}, \mathbf{P}'; \mathbf{Q}) \\ &\quad - \frac{\langle \mathbf{P} | \rho | \mathbf{P}' \rangle}{2} \int d\mathbf{Q} M_{\text{in}}(\mathbf{P} + \mathbf{Q}, \mathbf{P} + \mathbf{Q}; \mathbf{Q}) \\ &\quad - \frac{\langle \mathbf{P} | \rho | \mathbf{P}' \rangle}{2} \int d\mathbf{Q} M_{\text{in}}(\mathbf{P}' + \mathbf{Q}, \mathbf{P}' + \mathbf{Q}; \mathbf{Q}). \end{aligned} \quad (17)$$

The function $M_{\text{in}}(\mathbf{P}, \mathbf{P}'; \mathbf{Q})$ is defined below in Eq. (24) [see also (27) and (39)]. In order to highlight the relation to the classical linear Boltzmann equation, let us first note that the master equation takes the shorter form

$$\begin{aligned} \langle \mathbf{P} | \mathcal{L} \rho | \mathbf{P}' \rangle &= \int d\mathbf{Q} M_{\text{in}}(\mathbf{P}, \mathbf{P}'; \mathbf{Q}) \langle \mathbf{P} - \mathbf{Q} | \rho | \mathbf{P}' - \mathbf{Q} \rangle \\ &\quad - \frac{1}{2} [M_{\text{out}}^{\text{cl}}(\mathbf{P}) + M_{\text{out}}^{\text{cl}}(\mathbf{P}')] \langle \mathbf{P} | \rho | \mathbf{P}' \rangle \end{aligned} \quad (18)$$

once we introduce

$$M_{\text{out}}^{\text{cl}}(\mathbf{P}) := \int d\mathbf{Q} M_{\text{in}}(\mathbf{P} + \mathbf{Q}, \mathbf{P} + \mathbf{Q}; \mathbf{Q}). \quad (19)$$

As indicated by its name, this positive function gives the rate known from the *classical* linear Boltzmann equation [2] for a particle with momentum \mathbf{P} to be scattered to a different momentum. It involves an integration over all initial gas momenta \mathbf{p}_0 and all momentum exchanges \mathbf{Q} subject to the restriction implied by energy conservation,

$$\begin{aligned} M_{\text{out}}^{\text{cl}}(\mathbf{P}) &= \frac{n_{\text{gas}}}{m_*} \int d\mathbf{p}_0 d\mathbf{Q} \mu(\mathbf{p}_0) \\ &\quad \times \delta\left(\frac{|\text{rel}(\mathbf{p}_0, \mathbf{P})|^2 - |\text{rel}(\mathbf{p}_0, \mathbf{P}) + \mathbf{Q}|^2}{2}\right) \\ &\quad \times \sigma(\text{rel}(\mathbf{p}_0, \mathbf{P}) + \mathbf{Q}, \text{rel}(\mathbf{p}_0, \mathbf{P})). \end{aligned} \quad (20)$$

Here, μ is the gas momentum distribution function from (8), the function $\text{rel}(\mathbf{p}, \mathbf{P})$ is defined in (9), and σ is the differential cross section (15). Carrying out the \mathbf{Q} -integration one can write the rate in terms of the total cross section (16),

$$\begin{aligned} M_{\text{out}}^{\text{cl}}(\mathbf{P}) &= \frac{n_{\text{gas}}}{m_*} \int d\mathbf{p}_0 \mu(\mathbf{p}_0) |\text{rel}(\mathbf{p}_0, \mathbf{P})| \\ &\quad \times \sigma_{\text{tot}}(\text{rel}(\mathbf{p}_0, \mathbf{P})). \end{aligned} \quad (21)$$

It follows that the dynamics described by the “loss term” in (17), (18) is fully specified by the rate in the corresponding classical equation (which involves of course a quantum mechanical cross section). The term leads to a reduction of the momentum coherences $\langle \mathbf{P} | \rho | \mathbf{P}' \neq \mathbf{P} \rangle$ with a rate given by the arithmetic mean of the loss rates of the corresponding diagonal elements, $\langle \mathbf{P} | \rho | \mathbf{P} \rangle$ and

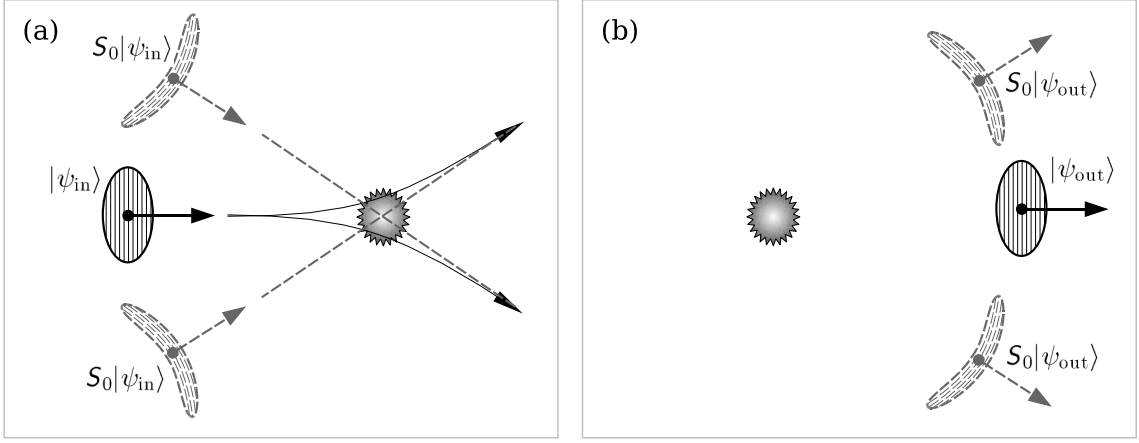


FIG. 1: Action of the S-matrix when applied to localized wave packets of the incoming and the outgoing type. (a) An incoming wave packet $|\psi_{\text{in}}\rangle$ is transformed in such a way that the free motion of the resulting state $S_0|\psi_{\text{in}}\rangle$ (indicated by the dashed curves) converges with the dynamically scattered wave packet at large times [20]. (b) An outgoing wave packet, whose forward time evolution will be unaffected by the scattering potential, gets strongly transformed by S_0 . This is due to the inverse time evolution involved in the definition of the the S-matrix. To prevent this unwanted transformation one should (i) either attribute a vanishing collision rate to all outgoing states or (ii) modify the S_0 operator such that it leaves all outgoing wave packets unaffected. Evaluations of $\mathcal{L}\rho$ based on these two strategies are given in Sect. V and Sect. VI, respectively.

$\langle \mathbf{P}' | \rho | \mathbf{P}' \rangle$, and these momentum populations, in turn, are depleted in the same way as the momentum distribution function of the classical linear Boltzmann equation.

The “gain term” in (17), (18) is also related to the classical linear Boltzmann equation, but only on the diagonal $\mathbf{P} = \mathbf{P}'$. As one expects, M_{in} is positive on the diagonal, and equal to the rate density $M_{\text{in}}^{\text{cl}}$ from the classical linear Boltzmann equation for the tracer particle to end up in momentum \mathbf{P}_f after a momentum gain of \mathbf{Q} ,

$$\begin{aligned}
 M_{\text{in}}^{\text{cl}}(\mathbf{P}_f; \mathbf{Q}) &= M_{\text{in}}(\mathbf{P}_f, \mathbf{P}_f; \mathbf{Q}) \equiv M^{\text{cl}}(\mathbf{P}_f - \mathbf{Q} \rightarrow \mathbf{P}_f) \\
 &= \frac{n_{\text{gas}}}{m_*} \int d\mathbf{p}_0 \mu(\mathbf{p}_0) \\
 &\quad \times \delta\left(\frac{|\text{rel}(\mathbf{p}_0 - \mathbf{Q}, \mathbf{P}_f)|^2 - |\text{rel}(\mathbf{p}_0, \mathbf{P}_f - \mathbf{Q})|^2}{2}\right) \\
 &\quad \times \sigma(\text{rel}(\mathbf{p}_0 - \mathbf{Q}, \mathbf{P}_f), \text{rel}(\mathbf{p}_0, \mathbf{P}_f - \mathbf{Q})). \quad (22)
 \end{aligned}$$

The second equality in (22) introduces the notation

$$M^{\text{cl}}(\mathbf{P}_i \rightarrow \mathbf{P}_f) := M_{\text{in}}^{\text{cl}}(\mathbf{P}_f; \mathbf{P}_f - \mathbf{P}_i), \quad (23)$$

for the rate density corresponding to a change of momentum \mathbf{P}_i to \mathbf{P}_f . It will be useful for the discussion of the classical linear Boltzmann equation in Sect. IX, and it yields the classical out rate (19) as $M_{\text{out}}^{\text{cl}}(\mathbf{P}) = \int d\mathbf{P}_f M^{\text{cl}}(\mathbf{P} \rightarrow \mathbf{P}_f)$ thus ensuring the conservation of probability.

For $\mathbf{P} \neq \mathbf{P}'$ the function M_{in} is in general complex-valued, and it has a rather complicated form when stated with its explicit dependence on \mathbf{P} , \mathbf{P}' , and \mathbf{Q} :

$$\begin{aligned}
 M_{\text{in}}(\mathbf{P}, \mathbf{P}'; \mathbf{Q}) &= \frac{n_{\text{gas}}}{m_*} \int d\mathbf{p}_0 \mu^{1/2} \left(\mathbf{p}_0 + \frac{m}{M} \frac{\mathbf{P}_{\parallel} - \mathbf{P}'_{\parallel}}{2} \right) \mu^{1/2} \left(\mathbf{p}_0 - \frac{m}{M} \frac{\mathbf{P}_{\parallel} - \mathbf{P}'_{\parallel}}{2} \right) \\
 &\quad \times f \left(\text{rel} \left(\mathbf{p}_0 - \mathbf{Q}, \mathbf{P} - \frac{\mathbf{P}_{\parallel} - \mathbf{P}'_{\parallel}}{2} \right), \text{rel} \left(\mathbf{p}_0, \mathbf{P} - \frac{\mathbf{P}_{\parallel} - \mathbf{P}'_{\parallel}}{2} - \mathbf{Q} \right) \right) \\
 &\quad \times f^* \left(\text{rel} \left(\mathbf{p}_0 - \mathbf{Q}, \mathbf{P}' + \frac{\mathbf{P}_{\parallel} - \mathbf{P}'_{\parallel}}{2} \right), \text{rel} \left(\mathbf{p}_0, \mathbf{P}' + \frac{\mathbf{P}_{\parallel} - \mathbf{P}'_{\parallel}}{2} - \mathbf{Q} \right) \right) \\
 &\quad \times \delta \left(\frac{\text{rel}(\mathbf{p}_0 - \mathbf{Q}, \frac{\mathbf{P} + \mathbf{P}'}{2})^2 - \text{rel}(\mathbf{p}_0, \frac{\mathbf{P} + \mathbf{P}'}{2} - \mathbf{Q})^2}{2} \right). \quad (24)
 \end{aligned}$$

Here we used the abbreviations

$$\mathbf{P}_{\parallel} := \frac{\mathbf{P} \cdot \mathbf{Q}}{Q^2} \mathbf{Q} \quad (25)$$

and

$$\mathbf{P}'_{\parallel} := \frac{\mathbf{P}' \cdot \mathbf{Q}}{Q^2} \mathbf{Q} \quad (26)$$

for the contributions in \mathbf{P} and \mathbf{P}' parallel to the momentum exchange $\mathbf{Q} \neq 0$. This form of $M_{\text{in}}(\mathbf{P}, \mathbf{P}'; \mathbf{Q})$ clearly reduces to the diagonal expression (22) when \mathbf{P} approaches \mathbf{P}' . The curious appearance of the \mathbf{P}_{\parallel} and \mathbf{P}'_{\parallel} contributions in (24) ensures, in combination with the delta-function, that the modulus of the initial and the final relative momentum are equal in both scattering amplitudes. This will be more obvious below in Sect. IV, where suitable relative coordinates are introduced. The energy conservation is thus manifestly guaranteed for each of the scattering amplitudes separately, while the arguments will differ in general.

One of the important properties of the “complex rate” (24) is that it admits a factorization of the \mathbf{P} - and \mathbf{P}' -dependence, which will be crucial later on, when we formulate the master equation in its representation-independent “operator form”. Specifically, it will be shown in Sect. VIII that M_{in} can be written as a two-dimensional integration over the set $\mathbf{Q}^{\perp} = \{\mathbf{p} \in \mathbb{R}^3 : \mathbf{p} \cdot \mathbf{Q} = 0\}$ of momenta perpendicular to the momentum exchange \mathbf{Q} . This way the integrand factorizes into a product of \mathbf{P} - and \mathbf{P}' -dependent terms,

$$M_{\text{in}}(\mathbf{P}, \mathbf{P}'; \mathbf{Q}) = \int_{\mathbf{Q}^{\perp}} d\mathbf{p} L(\mathbf{p}, \mathbf{P} - \mathbf{Q}; \mathbf{Q}) \times L^*(\mathbf{p}, \mathbf{P}' - \mathbf{Q}; \mathbf{Q}). \quad (27)$$

The functions

$$\begin{aligned} L(\mathbf{p}, \mathbf{P}; \mathbf{Q}) & \quad (28) \\ &= \sqrt{\frac{n_{\text{gas}} m}{Q m_*^2}} \mu \left(\mathbf{p}_{\perp \mathbf{Q}} + \left(1 + \frac{m}{M}\right) \frac{\mathbf{Q}}{2} + \frac{m}{M} \mathbf{P}_{\parallel \mathbf{Q}} \right)^{1/2} \\ & \times f \left(\text{rel}(\mathbf{p}_{\perp \mathbf{Q}}, \mathbf{P}_{\perp \mathbf{Q}}) - \frac{\mathbf{Q}}{2}, \text{rel}(\mathbf{p}_{\perp \mathbf{Q}}, \mathbf{P}_{\perp \mathbf{Q}}) + \frac{\mathbf{Q}}{2} \right), \end{aligned}$$

involve \mathbf{P}_{\parallel} defined in (25) and $\mathbf{P}_{\perp \mathbf{Q}} := \mathbf{P} - \mathbf{P}_{\parallel \mathbf{Q}}$. In the representation-independent form of the master equation they turn into operator-valued expressions, see Sect. VIII.

Concerning the coherent modification of the QLBE, it will be shown in Sect. VII that the momentum representation of the corresponding term (5) reads

$$\langle \mathbf{P} | \mathcal{R} \rho | \mathbf{P}' \rangle = \frac{E_{\text{n}}(\mathbf{P}) - E_{\text{n}}(\mathbf{P}')}{i\hbar} \langle \mathbf{P} | \rho | \mathbf{P}' \rangle \quad (29)$$

with

$$E_{\text{n}}(\mathbf{P}) = -2\pi\hbar^2 \frac{n_{\text{gas}}}{m_*} \int d\mathbf{p}_0 \mu(\mathbf{p}_0) \times \text{Re}[f(\text{rel}(\mathbf{p}_0, \mathbf{P}), \text{rel}(\mathbf{p}_0, \mathbf{P}))]. \quad (30)$$

This shows how the presence of the gas changes the energy of the particle with respect to the vacuum. This energy shift depends on the particle momentum and is determined by the real part of the average *forward* scattering amplitude. This phenomenon is well known in the field of neutron and atom interference, and it is usually accounted for by introducing an index of refraction, see Sect. IX E.

IV. EVALUATION IN THE MOMENTUM BASIS

A. Transformation to relative coordinates

Our main task in deriving the quantum linear Boltzmann equation is to evaluate the expressions (4) and (5), which is best done in the momentum representation. Starting with the incoherent part $\mathcal{L}\rho$, the cyclicity under the trace yields

$$\begin{aligned} \langle \mathbf{P} | \mathcal{L} \rho | \mathbf{P}' \rangle &= \int d\mathbf{Q} d\mathbf{Q}' \langle \mathbf{P} - \mathbf{Q} | \rho | \mathbf{P}' - \mathbf{Q}' \rangle M(\mathbf{P}, \mathbf{P}'; \mathbf{Q}, \mathbf{Q}') \\ & \quad - \frac{1}{2} \int d\mathbf{P}_0 \langle \mathbf{P}_0 | \rho | \mathbf{P}' \rangle \int d\mathbf{P}_f M(\mathbf{P}_f, \mathbf{P}_f; \mathbf{P}_f - \mathbf{P}_0, \mathbf{P}_f - \mathbf{P}) \\ & \quad - \frac{1}{2} \int d\mathbf{P}'_0 \langle \mathbf{P} | \rho | \mathbf{P}'_0 \rangle \int d\mathbf{P}_f M(\mathbf{P}_f, \mathbf{P}_f; \mathbf{P}_f - \mathbf{P}', \mathbf{P}_f - \mathbf{P}'_0) \end{aligned}$$

with

$$M(\mathbf{P}, \mathbf{P}'; \mathbf{Q}, \mathbf{Q}') = \langle \mathbf{P} | \text{Tr}_{\text{gas}} \left(\mathbb{T} \Gamma^{1/2} [|\mathbf{P} - \mathbf{Q}\rangle \langle \mathbf{P}' - \mathbf{Q}'| \otimes \rho_{\text{gas}}] \Gamma^{1/2} \mathbb{T}^\dagger \right) | \mathbf{P}' \rangle. \quad (31)$$

Upon inserting the stationary gas state (8) into (31) we can simplify the expression by transforming from the two-particle coordinates to the center-of-mass and relative coordinates using (10). Since Γ and T depend only on the relative motion, see (11) and (13), one thus finds

$$\begin{aligned} M(\mathbf{P}, \mathbf{P}'; \mathbf{Q}, \mathbf{Q}') &= \delta(\mathbf{Q} - \mathbf{Q}') \frac{(2\pi\hbar)^3}{|\Omega|} \int d\mathbf{p}_0 \mu(\mathbf{p}_0) \\ &\quad \times \langle \text{rel}(\mathbf{p}_0 - \mathbf{Q}, \mathbf{P}) | \mathsf{T}_0 \Gamma_0^{1/2} | \text{rel}(\mathbf{p}_0, \mathbf{P} - \mathbf{Q}) \rangle \\ &\quad \times \langle \text{rel}(\mathbf{p}_0, \mathbf{P}' - \mathbf{Q}) | \Gamma_0^{1/2} \mathsf{T}_0^\dagger | \text{rel}(\mathbf{p}_0 - \mathbf{Q}, \mathbf{P}') \rangle \\ &=: \delta(\mathbf{Q} - \mathbf{Q}') M_{\text{in}}(\mathbf{P}, \mathbf{P}'; \mathbf{Q}), \end{aligned} \quad (32)$$

as anticipated above in (17).

It is now helpful to introduce functions of \mathbf{p}_0 ,

$$\mathbf{p}_i = \text{rel}\left(\mathbf{p}_0, \frac{\mathbf{P} + \mathbf{P}'}{2} - \mathbf{Q}\right) \quad (33)$$

$$\mathbf{p}_f = \text{rel}\left(\mathbf{p}_0 - \mathbf{Q}, \frac{\mathbf{P} + \mathbf{P}'}{2}\right), \quad (34)$$

which denote the *mean* of the pairs of initial and final relative momenta appearing in (32). We also set

$$\mathbf{q} = \text{rel}\left(0, \frac{\mathbf{P} - \mathbf{P}'}{2}\right). \quad (35)$$

These definitions imply the relations

$$\begin{aligned} \mathbf{p}_f + \mathbf{q} &= \text{rel}(\mathbf{p}_0 - \mathbf{Q}, \mathbf{P}) \\ \mathbf{p}_f - \mathbf{q} &= \text{rel}(\mathbf{p}_0 - \mathbf{Q}, \mathbf{P}') \\ \mathbf{p}_i + \mathbf{q} &= \text{rel}(\mathbf{p}_0, \mathbf{P} - \mathbf{Q}) \\ \mathbf{p}_i - \mathbf{q} &= \text{rel}(\mathbf{p}_0, \mathbf{P}' - \mathbf{Q}) \\ \mathbf{p}_i - \mathbf{p}_f &= \mathbf{Q}, \end{aligned} \quad (36)$$

which are noted here for later reference. Moreover, for given \mathbf{q} we shall write

$$\mathbf{q}_{\parallel} \equiv \frac{\mathbf{q} \cdot (\mathbf{p}_f - \mathbf{p}_i)}{(\mathbf{p}_f - \mathbf{p}_i)^2} (\mathbf{p}_f - \mathbf{p}_i) \quad (37)$$

$$\mathbf{q}_{\perp} \equiv \mathbf{q} - \mathbf{q}_{\parallel} \quad (38)$$

to denote the components parallel and perpendicular to the momentum exchange $\mathbf{Q} = \mathbf{p}_i - \mathbf{p}_f$.

The complex rate density defined in the second equality of (32) now takes the form

$$\begin{aligned} M_{\text{in}}(\mathbf{P}, \mathbf{P}'; \mathbf{Q}) &= \int d\mathbf{p}_0 \mu(\mathbf{p}_0) \frac{(2\pi\hbar)^3}{|\Omega|} \\ &\quad \times \langle \mathbf{p}_f + \mathbf{q} | \mathsf{T}_0 \Gamma_0^{1/2} | \mathbf{p}_i + \mathbf{q} \rangle \\ &\quad \times \langle \mathbf{p}_i - \mathbf{q} | \Gamma_0^{1/2} \mathsf{T}_0^\dagger | \mathbf{p}_f - \mathbf{q} \rangle. \end{aligned}$$

We can write it as the average over the gas momentum distribution function μ of a rate density in the center-of-mass frame,

$$M_{\text{in}}(\mathbf{P}, \mathbf{P}'; \mathbf{Q}) = \int d\mathbf{p}_0 \mu(\mathbf{p}_0) m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}), \quad (39)$$

thus formally introducing

$$\begin{aligned} m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}) &= \frac{(2\pi\hbar)^3}{|\Omega|} \langle \mathbf{p}_f + \mathbf{q} | \mathsf{T}_0 \Gamma_0^{1/2} | \mathbf{p}_i + \mathbf{q} \rangle \\ &\quad \times \langle \mathbf{p}_i - \mathbf{q} | \Gamma_0^{1/2} \mathsf{T}_0^\dagger | \mathbf{p}_f - \mathbf{q} \rangle \end{aligned} \quad (40)$$

in terms of matrix elements of $\mathsf{T}_0 \Gamma_0^{1/2}$ with respect to the relative momentum coordinates. This expression should be viewed here as a generalized function in the sense of distributions, with independent variables $\mathbf{p}_f, \mathbf{p}_i$, and \mathbf{q} .

The main aim of the following sections is to show, in two independent lines of argument, that the expression (40) should be understood as

$$m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}) = \begin{cases} m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}_{\perp}) & \text{if } \mathbf{q} \cdot (\mathbf{p}_f - \mathbf{p}_i) = 0 \\ 0 & \text{otherwise,} \end{cases} \quad (41)$$

with

$$\begin{aligned} m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}_{\perp}) &= \frac{n_{\text{gas}}}{m_*} \delta\left(\frac{\mathbf{p}_f^2 - \mathbf{p}_i^2}{2}\right) f(\mathbf{p}_f + \mathbf{q}_{\perp}, \mathbf{p}_i + \mathbf{q}_{\perp}) \\ &\quad \times f^*(\mathbf{p}_f - \mathbf{q}_{\perp}, \mathbf{p}_i - \mathbf{q}_{\perp}). \end{aligned} \quad (42)$$

Note that this term involves a single delta-function and the abbreviation \mathbf{q}_{\perp} just defined in (38).

B. Diagonal evaluation of the trace

As a first step, let us try to evaluate (40) in a straightforward fashion by maintaining that the operator Γ_0 is diagonal in the relative momentum coordinates. Equation (12) then implies

$$\Gamma_0^{1/2} |\mathbf{p}\rangle = \sqrt{\Gamma_0(\mathbf{p})} |\mathbf{p}\rangle \quad (43)$$

with

$$\Gamma_0(\mathbf{p}) := \frac{n_{\text{gas}}}{m_*} |\mathbf{p}| \sigma_{\text{tot}}(\mathbf{p}). \quad (44)$$

Noting that the T_0 matrix elements are given by (14) one thus obtains the generalized function

$$\begin{aligned} m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}) &= \Gamma_0^{1/2}(\mathbf{p}_i + \mathbf{q}) \Gamma_0^{1/2}(\mathbf{p}_i - \mathbf{q}) \\ &\quad \times f(\mathbf{p}_f + \mathbf{q}, \mathbf{p}_i + \mathbf{q}) f^*(\mathbf{p}_f - \mathbf{q}, \mathbf{p}_i - \mathbf{q}) \\ &\quad \times \frac{2\pi\hbar}{|\Omega|} \delta\left(\frac{\mathbf{p}_f^2 - \mathbf{p}_i^2}{2} + (\mathbf{p}_f - \mathbf{p}_i) \cdot \mathbf{q}\right) \\ &\quad \times \delta\left(\frac{\mathbf{p}_f^2 - \mathbf{p}_i^2}{2} - (\mathbf{p}_f - \mathbf{p}_i) \cdot \mathbf{q}\right). \end{aligned} \quad (45)$$

Clearly, the two delta-functions ensure that the energy is conserved in each of the “elastic collision trajectories” expressed by the arguments of the two scattering amplitudes in (45). Employing the relation

$\delta(a + b/2) \delta(a - b/2) = \delta(a) \delta(b)$ we obtain the equivalent form

$$m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}) = \delta\left(\frac{\mathbf{p}_f^2 - \mathbf{p}_i^2}{2}\right) \Gamma_0^{1/2}(\mathbf{p}_i + \mathbf{q}) \Gamma_0^{1/2}(\mathbf{p}_i - \mathbf{q}) \\ \times f(\mathbf{p}_f + \mathbf{q}, \mathbf{p}_i + \mathbf{q}) f^*(\mathbf{p}_f - \mathbf{q}, \mathbf{p}_i - \mathbf{q}) \\ \times \delta((\mathbf{p}_f - \mathbf{p}_i) \cdot \mathbf{q}) \frac{\pi \hbar}{|\Omega|}. \quad (46)$$

The first delta function now requires \mathbf{p}_i and \mathbf{p}_f to have equal length. These are the mean relative momenta of the pairs of scattering trajectories, as defined in Eqs. (33) and (34). Given $|\mathbf{p}_i| = |\mathbf{p}_f|$, the second delta function ensures that the energy is conserved in each of the scattering amplitudes individually, by granting that \mathbf{q} , which expresses a “distance” between the two pairs of scattering trajectories, is orthogonal to the momentum exchange $\mathbf{p}_i - \mathbf{p}_f$. The fact that possible parallel components of $\mathbf{q} = \mathbf{q}_\perp + \mathbf{q}_\parallel$ cannot contribute to an integral over the generalized function (46) can be made manifest by replacing the \mathbf{q} ’s outside of the delta function by the orthogonal component \mathbf{q}_\perp defined in (38). In other words, the statement (46) is tantamount to

$$m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}) \\ = \delta\left(\frac{\mathbf{p}_f^2 - \mathbf{p}_i^2}{2}\right) \Gamma_0^{1/2}(\mathbf{p}_i + \mathbf{q}_\perp) \Gamma_0^{1/2}(\mathbf{p}_i - \mathbf{q}_\perp) \\ \times f(\mathbf{p}_f + \mathbf{q}_\perp, \mathbf{p}_i + \mathbf{q}_\perp) f^*(\mathbf{p}_f - \mathbf{q}_\perp, \mathbf{p}_i - \mathbf{q}_\perp) \\ \times \delta((\mathbf{p}_f - \mathbf{p}_i) \cdot \mathbf{q}) \frac{\pi \hbar}{|\Omega|}, \quad (47)$$

which implies that the expression vanishes for $\mathbf{q}_\parallel \neq 0$, as stated in (41). In fact, even if the integration over m_{in} involves a smooth function $g(\mathbf{q})$ the second delta function will enforce that the latter contributes only with the orthogonal component of \mathbf{q} ,

$$m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}) g(\mathbf{q}) = m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}_\perp) g(\mathbf{q}_\perp). \quad (48)$$

One observes on the right hand side of (47) that already the first two lines now manifestly ensure the energy conservation of the pair of collision trajectories described by the two scattering amplitudes. This is a crucial requirement since the scattering amplitudes are not defined off the energy shell (notwithstanding the fact that analytic continuations are often considered and helpful in scattering theory). At the same time this implies that the physical relevance of the second delta-function has been accounted for once the parallel components of \mathbf{q} have been set to zero. Hence, the third line in (47) is essentially dispensable, which is all the more important since it renders m_{in} an ill-defined expression due to the appearance of the arbitrarily large normalization volume $|\Omega|$.

As is well understood, the evaluation carried out in this subsection does not yield a well-behaved result because it

takes the momentum-diagonal form (12) of the rate operator Γ too seriously. It was already discussed in Sect. IIB that either Γ should involve a projection to the subspace of incoming wave packets, or that the operator S should be redefined such that it keeps the outgoing wave packets unchanged. These two strategies will be implemented in Sects. V and VI, yielding identical results. As one expects, the overall structure of (47), which is dictated by the energy conservation, will not change, but the third line will be replaced by a proper normalization.

V. WAVE PACKET EVALUATION

The aim of this section is to evaluate the generalized function

$$m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}_\perp) = \frac{(2\pi\hbar)^3}{|\Omega|} \langle \mathbf{p}_f + \mathbf{q}_\perp | \Gamma_0^{1/2} | \mathbf{p}_i + \mathbf{q}_\perp \rangle \\ \times \langle \mathbf{p}_i - \mathbf{q}_\perp | \Gamma_0^{1/2} \Gamma_0^\dagger | \mathbf{p}_f - \mathbf{q}_\perp \rangle \quad (49)$$

by consistently incorporating the fact that the rate operator Γ_0 should have a vanishing expectation value for those states of the relative motion that are not of incoming type. As a first step, we will write (49) as the expectation value of a non-hermitian operator with respect to a properly normalized momentum state of the relative motion. For that purpose it is convenient to introduce the operator $Z_0 := \Gamma_0 \Gamma_0^{1/2}$ and its translation by the momentum \mathbf{q}_\perp ,

$$Z_{\mathbf{q}_\perp} = \exp\left(-i \frac{\mathbf{x}_{\text{rel}} \cdot \mathbf{q}_\perp}{\hbar}\right) \Gamma_0 \Gamma_0^{1/2} \exp\left(i \frac{\mathbf{x}_{\text{rel}} \cdot \mathbf{q}_\perp}{\hbar}\right) \quad (50)$$

where \mathbf{x}_{rel} is the position operator of the relative coordinate. Moreover, we note that, analogous to (7), a volume-normalized momentum state of the *relative* motion has the form

$$\rho_{\mathbf{p}_i} = \frac{(2\pi\hbar)^3}{|\Omega|} |\Omega| |\mathbf{p}_i\rangle \langle \mathbf{p}_i|. \quad (51)$$

Combining (50) and (51) one finds that the complex rate density (49) can be taken as the diagonal momentum matrix element of an operator product, $m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}_\perp) = \langle \mathbf{p}_f | Z_{\mathbf{q}_\perp} \rho_{\mathbf{p}_i} Z_{-\mathbf{q}_\perp}^\dagger | \mathbf{p}_f \rangle$, provided the projection to the normalization volume is included. If we further denote the projector to improper momentum eigenstates as $\mathbf{P}_{\mathbf{p}_f} = |\mathbf{p}_f\rangle \langle \mathbf{p}_f|$ we can write

$$m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}_\perp) = \text{Tr}\left(Z_{-\mathbf{q}_\perp}^\dagger \mathbf{P}_{\mathbf{p}_f} Z_{\mathbf{q}_\perp} \rho_{\mathbf{p}_i}\right). \quad (52)$$

The complex rate density (49) has now the form of an expectation value with respect to a state $\rho_{\mathbf{p}_i}$ which is properly normalized, $\text{Tr}(\rho_{\mathbf{p}_i}) = 1$. As discussed in Sect. IIB, the rate operator Γ_0 , and therefore also the non-hermitian operator $Z_{-\mathbf{q}_\perp}^\dagger \mathbf{P}_{\mathbf{p}_f} Z_{\mathbf{q}_\perp}$ should include a restriction to the subspace of truly incoming relative motional

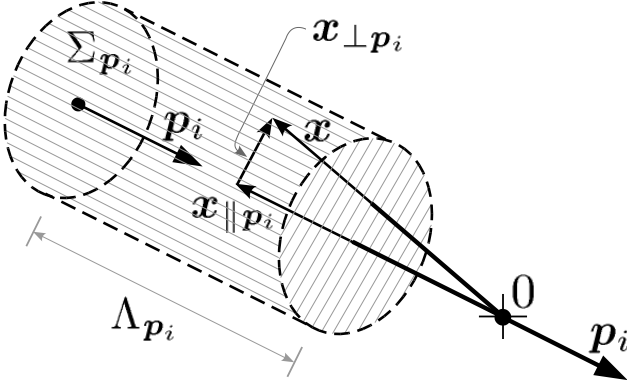


FIG. 2: The incoming relative momentum \mathbf{p}_i defines a cylinder with base area $\Sigma_{\mathbf{p}_i}$ and height $\Lambda_{\mathbf{p}_i}$. This spatial region is used to implement the phase space restriction of the Wigner function to incoming states.

states. Starting from (52), one can now implement this restriction in a rather transparent and intuitive fashion by considering the phase space representation of $\rho_{\mathbf{p}_i}$, as shown in the next subsection. A similar method was already successfully applied in [9], where the effect of a gas on the internal dynamics of an immobile system was discussed by combining the monitoring approach with scattering theory.

A. Phase space restriction to incoming wave packets

The operator $\rho_{\mathbf{p}_i}$ in (52) characterizes the motional state of the relative coordinates between particle and gas prior to a collision. According to (51) it is given by a plane wave which extends through the whole normalization volume, and it is therefore clearly not of the incoming type required for the application of scattering theory.

The Wigner-Weyl formulation of quantum mechanics [21, 22, 23, 24] suggests a way to treat this problem. Continuous variable states may be represented by the phase space quasi-probability function $W_\rho(\mathbf{x}, \mathbf{p}) := (2\pi\hbar)^{-3} \int d\mathbf{q} \exp(-i\mathbf{q} \cdot \mathbf{x}/\hbar) \langle \mathbf{p} - \mathbf{q}/2 | \rho | \mathbf{p} + \mathbf{q}/2 \rangle$. For the state (51) the associated Wigner function reads³

$$W_{\mathbf{p}_i}(\mathbf{x}, \mathbf{p}) = \frac{\chi_\Omega(\mathbf{x})}{|\Omega|} \delta(\mathbf{p} - \mathbf{p}_i), \quad (53)$$

where χ_Ω is the characteristic function of the normalization volume $|\Omega|$. Given that expectation values like (52) may now be calculated as phase space integrals, it is natural to implement the restriction by confining (53) to the

phase space area of incoming wave packets, i.e.,

$$W'_{\mathbf{p}_i}(\mathbf{x}, \mathbf{p}) = \frac{\chi_{\Lambda_{\mathbf{p}_i}}(\mathbf{x}_{\parallel \mathbf{p}_i})}{|\Lambda_{\mathbf{p}_i}|} \frac{\chi_{\Sigma_{\mathbf{p}_i}}(\mathbf{x}_{\perp \mathbf{p}_i})}{|\Sigma_{\mathbf{p}_i}|} \delta(\mathbf{p} - \mathbf{p}_i) \quad (54)$$

Here, the product $\chi_{\Lambda_{\mathbf{p}_i}}(\mathbf{x}_{\parallel \mathbf{p}_i}) \chi_{\Sigma_{\mathbf{p}_i}}(\mathbf{x}_{\perp \mathbf{p}_i})$ is the characteristic function of a cylinder pointing towards the origin, see Fig. 2. It describes those points $\mathbf{x} = \mathbf{x}_{\parallel \mathbf{p}_i} + \mathbf{x}_{\perp \mathbf{p}_i}$ in position space which will pass the vicinity of the origin when propagated in the direction given by \mathbf{p}_i . $\Sigma_{\mathbf{p}_i}$ is the base surface of the cylinder and its area will be taken to be equal to the total cross section below, i.e., $|\Sigma_{\mathbf{p}_i}| = \sigma(\mathbf{p}_i)$. The interval $\Lambda_{\mathbf{p}_i}$ specifies the cylinder height; its precise \mathbf{p}_i -dependence will drop out of the calculation later on.

The operator corresponding to (54) reads

$$\rho'_{\mathbf{p}_i} = \int_{\Lambda_{\mathbf{p}_i}} \frac{d\mathbf{x}_{\parallel \mathbf{p}_i}}{|\Lambda_{\mathbf{p}_i}|} \int_{\Sigma_{\mathbf{p}_i}} \frac{d\mathbf{x}_{\perp \mathbf{p}_i}}{|\Sigma_{\mathbf{p}_i}|} \int d\mathbf{w} \times \exp\left(i\frac{\mathbf{x} \cdot \mathbf{w}}{\hbar}\right) |\mathbf{p}_i - \frac{\mathbf{w}}{2}\rangle \langle \mathbf{p}_i + \frac{\mathbf{w}}{2}|, \quad (55)$$

so that compared to the unrestricted expression corresponding to (53)

$$\int_\Omega \frac{d\mathbf{x}}{|\Omega|} \int d\mathbf{w} \exp\left(i\frac{\mathbf{x} \cdot \mathbf{w}}{\hbar}\right) |\mathbf{p}_i - \frac{\mathbf{w}}{2}\rangle \langle \mathbf{p}_i + \frac{\mathbf{w}}{2}| \quad (56)$$

the spatial average over the whole normalization volume is simply replaced by an average over the cylinder, and the norm is indeed preserved,

$$\text{Tr}(\rho'_{\mathbf{p}_i}) = \int_{\Lambda_{\mathbf{p}_i}} \frac{d\mathbf{x}_{\parallel \mathbf{p}_i}}{|\Lambda_{\mathbf{p}_i}|} \int_{\Sigma_{\mathbf{p}_i}} \frac{d\mathbf{x}_{\perp \mathbf{p}_i}}{|\Sigma_{\mathbf{p}_i}|} = 1. \quad (57)$$

It should be noted, though, that strictly speaking neither $\rho_{\mathbf{p}_i}$ nor $\rho'_{\mathbf{p}_i}$ are legitimate quantum states since they combine a precise momentum with a finite position variance. They should rather be seen as convenient basis states admitting to average over the momentum distribution function, see Eqs. (8) and (39).

B. Restricted evaluation

Inserting the restricted state (55) into (52) one can now evaluate the complex rate density to obtain a well-defined expression. Starting with

$$\begin{aligned} m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}_\perp) &\cong \text{Tr}\left(Z_{-\mathbf{q}_\perp}^\dagger \mathbf{P}_{\mathbf{p}_f} Z_{\mathbf{q}_\perp} \rho'_{\mathbf{p}_i}\right) \\ &= \int_{\Lambda_{\mathbf{p}_i}} \frac{d\mathbf{x}_{\parallel \mathbf{p}_i}}{|\Lambda_{\mathbf{p}_i}|} \int_{\Sigma_{\mathbf{p}_i}} \frac{d\mathbf{x}_{\perp \mathbf{p}_i}}{|\Sigma_{\mathbf{p}_i}|} \int d\mathbf{w} \exp\left(i\frac{\mathbf{x} \cdot \mathbf{w}}{\hbar}\right) \\ &\quad \times \langle \mathbf{p}_f + \mathbf{q}_\perp | \mathbf{T}_0 \Gamma_0^{1/2} | \mathbf{p}_i + \mathbf{q}_\perp - \frac{\mathbf{w}}{2} \rangle \\ &\quad \times \langle \mathbf{p}_i - \mathbf{q}_\perp + \frac{\mathbf{w}}{2} | \Gamma_0^{1/2} \mathbf{T}_0^\dagger | \mathbf{p}_f - \mathbf{q}_\perp \rangle \end{aligned} \quad (58)$$

³ This follows with the approximation $\chi_\Omega(\mathbf{r} - \frac{\mathbf{s}}{2}) \chi_\Omega(\mathbf{r} + \frac{\mathbf{s}}{2}) \simeq \chi_\Omega(\mathbf{r}) \chi_\Omega(\mathbf{s})$, which is permissible since the normalization region Ω may be taken arbitrarily large.

we can now use with confidence the expressions (14) and (43) for the momentum matrix elements of T_0 and $\Gamma_0^{1/2}$. Thus, $m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}_\perp)$ takes the form

$$\begin{aligned}
m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}_\perp) &= \int_{\Lambda_{\mathbf{p}_i}} \frac{d\mathbf{x}_{\parallel \mathbf{p}_i}}{|\Lambda_{\mathbf{p}_i}|} \int_{\Sigma_{\mathbf{p}_i}} \frac{d\mathbf{x}_{\perp \mathbf{p}_i}}{|\Sigma_{\mathbf{p}_i}|} \int d\mathbf{w} \exp\left(-i \frac{\mathbf{x} \cdot \mathbf{w}}{\hbar}\right) \\
&\times \frac{1}{(2\pi\hbar)^2} f\left(\mathbf{p}_f + \mathbf{q}_\perp, \mathbf{p}_i + \mathbf{q}_\perp + \frac{\mathbf{w}}{2}\right) \\
&\times f^*\left(\mathbf{p}_f - \mathbf{q}_\perp, \mathbf{p}_i - \mathbf{q}_\perp - \frac{\mathbf{w}}{2}\right) \\
&\times \delta\left(\frac{\mathbf{p}_f^2 - \mathbf{p}_i^2}{2} - \frac{\mathbf{q}_\perp \cdot \mathbf{w}}{2} - \frac{w^2}{8} - \frac{1}{2} \mathbf{p}_i \cdot \mathbf{w}\right) \\
&\times \delta\left(\frac{\mathbf{p}_f^2 - \mathbf{p}_i^2}{2} - \frac{\mathbf{q}_\perp \cdot \mathbf{w}}{2} - \frac{w^2}{8} + \frac{1}{2} \mathbf{p}_i \cdot \mathbf{w}\right) \\
&\times \Gamma_0^{1/2}\left(\mathbf{p}_i + \mathbf{q}_\perp + \frac{\mathbf{w}}{2}\right) \Gamma_0^{1/2}\left(\mathbf{p}_i - \mathbf{q}_\perp - \frac{\mathbf{w}}{2}\right). \tag{59}
\end{aligned}$$

In the arguments of the delta function we took into account that \mathbf{q}_\perp is orthogonal to the momentum exchange, $(\mathbf{p}_f - \mathbf{p}_i) \cdot \mathbf{q}_\perp = 0$, as follows from (38). Using again the relation $\delta(a + b/2) \delta(a - b/2) = \delta(a) \delta(b)$ a delta function is obtained with argument $\mathbf{p}_i \cdot \mathbf{w}$. Writing $\mathbf{w} = \mathbf{w}_{\parallel \mathbf{p}_i} + \mathbf{w}_{\perp \mathbf{p}_i}$, with $\mathbf{w}_{\parallel \mathbf{p}_i} = (\mathbf{w} \cdot \mathbf{p}_i) \mathbf{p}_i / p_i^2$, this delta function renders $\mathbf{w}_{\parallel \mathbf{p}_i} = 0$, and as a result the integrand now no longer depends on $\mathbf{x}_{\parallel \mathbf{p}_i}$. It follows that the integration along the cylinder axis can be done, $\int_{\Lambda_{\mathbf{p}_i}} d\mathbf{x}_{\parallel \mathbf{p}_i} = |\Lambda_{\mathbf{p}_i}|$. We obtain

$$\begin{aligned}
m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}_\perp) &= \frac{n_{\text{gas}}}{m_*} \int d\mathbf{w} \delta\left(\frac{\mathbf{p}_i \cdot \mathbf{w}}{p_i}\right) \int_{\Sigma_{\mathbf{p}_i}} \frac{d\mathbf{x}_{\perp \mathbf{p}_i}}{(2\pi\hbar)^2} \\
&\times \exp\left(-i \frac{\mathbf{x}_{\perp \mathbf{p}_i} \cdot \mathbf{w}_{\perp \mathbf{p}_i}}{\hbar}\right) \\
&\times \delta\left(\frac{\mathbf{p}_f^2 - \mathbf{p}_i^2}{2} - \frac{\mathbf{q}_\perp \cdot \mathbf{w}}{2} - \frac{w^2}{8}\right) \\
&\times f\left(\mathbf{p}_f + \mathbf{q}_\perp, \mathbf{p}_i + \mathbf{q}_\perp + \frac{\mathbf{w}}{2}\right) \\
&\times f^*\left(\mathbf{p}_f - \mathbf{q}_\perp, \mathbf{p}_i - \mathbf{q}_\perp - \frac{\mathbf{w}}{2}\right) \\
&\times \frac{1}{p_i} \sqrt{\left|\mathbf{p}_i + \mathbf{q}_\perp + \frac{\mathbf{w}}{2}\right| \left|\mathbf{p}_i - \mathbf{q}_\perp - \frac{\mathbf{w}}{2}\right|} \\
&\times \frac{1}{\sigma_{\text{tot}}(\mathbf{p}_i)} \sqrt{\sigma_{\text{tot}}\left(\mathbf{p}_i + \mathbf{q}_\perp + \frac{\mathbf{w}}{2}\right)} \\
&\times \sqrt{\sigma_{\text{tot}}\left(\mathbf{p}_i - \mathbf{q}_\perp - \frac{\mathbf{w}}{2}\right)}, \tag{60}
\end{aligned}$$

where we identified the cylinder base area with the total cross section, $|\Sigma_{\mathbf{p}_i}| = \sigma_{\text{tot}}(\mathbf{p}_i)$. One observes that the $\mathbf{x}_{\perp \mathbf{p}_i}$ -integration over the surface $\Sigma_{\mathbf{p}_i}$ of the cylinder base yields an approximate two-dimensional delta function in

$\mathbf{w}_{\perp \mathbf{p}_i}$. Combined with the one-dimensional delta function in $w_{\parallel \mathbf{p}_i} = \mathbf{p}_i \cdot \mathbf{w} / p_i$ this gives a three-dimensional $\delta(\mathbf{w})$, which permits to carry out the \mathbf{w} -integration. We arrive at the well-defined expression

$$\begin{aligned}
m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}_\perp) &= \frac{n_{\text{gas}}}{m_*} \delta\left(\frac{\mathbf{p}_f^2 - \mathbf{p}_i^2}{2}\right) f(\mathbf{p}_f + \mathbf{q}_\perp, \mathbf{p}_i + \mathbf{q}_\perp) \\
&\times f^*(\mathbf{p}_f - \mathbf{q}_\perp, \mathbf{p}_i - \mathbf{q}_\perp) \\
&\times \frac{\sqrt{|\mathbf{p}_i + \mathbf{q}_\perp| |\mathbf{p}_i - \mathbf{q}_\perp|}}{p_i} \\
&\times \frac{\sqrt{\sigma_{\text{tot}}(\mathbf{p}_i + \mathbf{q}_\perp) \sigma_{\text{tot}}(\mathbf{p}_i - \mathbf{q}_\perp)}}{\sigma_{\text{tot}}(\mathbf{p}_i)}. \tag{61}
\end{aligned}$$

It shows that the complex rate density (39) is essentially given by the product of two scattering amplitudes whose arguments differ in general. They correspond to scattering “trajectories” determined by the relative momenta \mathbf{p}_i , \mathbf{p}_f , and \mathbf{q}_\perp . The \mathbf{p}_i and \mathbf{p}_f provide the arithmetic means of the initial and the final momenta, while \mathbf{q}_\perp characterizes the distance of the “trajectories” in momentum space. Since \mathbf{q}_\perp is orthogonal to $\mathbf{p}_f - \mathbf{p}_i$, a single delta-function suffices in (61) to ensure the conservation of energy in both scattering amplitudes.

Reassuringly, this result reduces to the classical rate density (22) for $\mathbf{q}_\perp = 0$, as can be seen easily by inserting $m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; 0)$ into (39). This shows that the first line in (61) may be viewed as a natural quantum generalization of the classical case, where the “off-diagonal” contributions with $\mathbf{q}_\perp \neq 0$ represent quantum corrections. From the point of view of quantum physics, there is indeed no reason why the effect of the gas collisions on the tracer particle should be confined to the “diagonal” contributions given by $\mathbf{q}_\perp = 0$. In the present relative coordinate representation, the first line in (61) has in fact a straightforward interpretation. It simply provides the contribution of the scattering amplitudes of any pair of scattering trajectories, which is allowed by both the energy conservation and the choice of \mathbf{P} , \mathbf{P}' , and \mathbf{Q} in (24).

At the same time, one expects that a \mathbf{q}_\perp -integration will average out the “far off-diagonal” contributions with large modulus $|\mathbf{q}_\perp|$, where the phases of the two scattering amplitudes are no longer synchronous. It is therefore reasonable to disregard the weak \mathbf{q}_\perp -dependence in the second line of (61), and this is corroborated by the fact that its linear dependence on \mathbf{q}_\perp vanishes identically. This removes the second line altogether, so that we end up with the form claimed in Eq. (42).

A noteworthy step in the present line of reasoning was that the base area $|\Sigma_{\mathbf{p}_i}|$ of the cylinder required for distinguishing the incoming states was identified with the scattering cross section σ_{tot} . This is very natural from a physical point of view, but it seems hard to justify on a formal basis. It is therefore worthwhile to present a second argumentation which, though very different in nature, leads to the identical result.

VI. EVALUATION WITH MODIFIED SCATTERING OPERATOR

A second, more heuristic approach of evaluating m_{in} sidesteps the issue of how to incorporate a restriction of the rate operator Γ_0 to the incoming wave packets, and takes its momentum-diagonal form (12) at face value. The unrestricted Γ_0 then attributes a finite scattering rate also to *outgoing* wave packets, which would never touch the interaction region in a dynamic description. This forces us to consider a redefinition of the scattering operator, which is necessary since outgoing wave packets are not left invariant by the proper S-matrix S_0 , as discussed above in Fig. 1. Let us therefore formally replace S_0 by a modified operator S'_0 , which by construction acts like S_0 when applied to asymptotic-in states, but leaves states with outgoing characteristics invariant. It will not be necessary to specify the details of this modification since all that is needed for the evaluation of m_{in} can be obtained from a single property that must hold for any such modified operator. It is the isometry of S'_0 with respect to the set of volume-normalized momentum states.

The advantage of replacing S_0 by S'_0 is that we can now use plane waves not merely as a basis, but as representing proper states, because the unwanted transformation of their outgoing components is now formally excluded. Like in Sect. II, we use double brackets to denote momentum states which are normalized with respect to the volume Ω and subject to periodic boundary conditions on its border. Due to the finite size of Ω they form a discrete basis $\{||\mathbf{p}\rangle\rangle : \mathbf{p} \in \mathbb{P}\}$, decomposing the identity (6) as

$$I_\Omega = \sum_{\mathbf{p} \in \mathbb{P}_\Omega} ||\mathbf{p}\rangle\rangle \langle\langle \mathbf{p}||. \quad (62)$$

Heuristically, one may view each $\mathbf{p} \in \mathbb{P}$ as labeling a distinct lead connected into and out of the scattering center. An important difference with respect to a continuous description is that the unitarity of the proper S-matrix, which expresses itself in the optical theorem, cannot be accommodated within this discrete setting. The optical theorem quantifies the diffraction limitation of the scattering cross section, telling ‘how much’ of a plane wave would pass the scattering center without distortion. If we describe the scattering process in terms of the amplitudes corresponding to discrete momentum states, or distinct leads, then the possibility of ‘passing the target’ is no longer available since any matrix element may have a finite amplitude. [The possibility of ‘forward scattering’ $||\mathbf{p}_i\rangle\rangle \rightarrow ||\mathbf{p}_i\rangle\rangle$ differs from this diffractive “passing” and leads to an additional phase shift, see the following section.] This suggests to disregard the identity operator in S'_0 , which relates to the unscattered part of the state, and to require of the remaining transition operator that it conserves the norm,

$$||S'_0||\mathbf{p}_i\rangle\rangle||^2 = ||T'_0||\mathbf{p}_i\rangle\rangle||^2 = 1. \quad (63)$$

Inserting the identity (62) we see that the sum of the probabilities of scattering into the different leads equals 1,

$$\sum_{\mathbf{p} \in \mathbb{P}_\Omega} | \langle\langle \mathbf{p} | T'_0 | \mathbf{p}_i \rangle\rangle |^2 = 1. \quad (64)$$

This is the standard property of the transition matrix used to describe discrete scattering problems between a finite number of incoming and outgoing leads, e.g. in mesoscopic physics [25] or the field of quantum graphs [26]. It seems natural to demand this relation of any reasonably modified operator T'_0 .

The use of (64) is that it tells us how to normalize the square of T'_0 matrix elements with respect to improper momentum kets. Inspecting the momentum matrix element of the T_0 operator given in (14) one finds that $| \langle\langle \mathbf{p}_f | T_0 | \mathbf{p}_i \rangle\rangle |^2$ involves the square of a delta-function. The expression should be well-defined when using the modified operator T'_0 , and the obvious choice is to assume that it is given by the corresponding expression with a single delta-function and a normalization $\mathcal{N}(\mathbf{p}_i)$ yet to be specified,

$$\frac{(2\pi\hbar)^3}{|\Omega|} | \langle\langle \mathbf{p}_f | T'_0 | \mathbf{p}_i \rangle\rangle |^2 = \mathcal{N}(\mathbf{p}_i) \delta\left(\frac{\mathbf{p}_f^2 - \mathbf{p}_i^2}{2}\right) |f(\mathbf{p}_f, \mathbf{p}_i)|^2. \quad (65)$$

Approximating the summation in (64) by the corresponding integral one finds

$$\begin{aligned} 1 &= \int d\mathbf{p}_f \frac{(2\pi\hbar)^3}{|\Omega|} | \langle\langle \mathbf{p}_f | T'_0 | \mathbf{p}_i \rangle\rangle |^2 \\ &= \mathcal{N}(\mathbf{p}_i) \int d\mathbf{p}_f \delta\left(\frac{\mathbf{p}_f^2 - \mathbf{p}_i^2}{2}\right) |f(\mathbf{p}_f, \mathbf{p}_i)|^2 \\ &= \mathcal{N}(\mathbf{p}_i) |\mathbf{p}_i|_{\sigma_{\text{tot}}}(\mathbf{p}_i). \end{aligned}$$

This fixes the normalization, $\mathcal{N}(\mathbf{p}_i) = [|\mathbf{p}_i|_{\sigma_{\text{tot}}}(\mathbf{p}_i)]^{-1}$ and we obtain a well-defined expression for the squared matrix element of the modified operator T'_0 ,

$$\frac{(2\pi\hbar)^3}{|\Omega|} | \langle\langle \mathbf{p}_f | T'_0 | \mathbf{p}_i \rangle\rangle |^2 = \delta\left(\frac{\mathbf{p}_f^2 - \mathbf{p}_i^2}{2}\right) \frac{|f(\mathbf{p}_f, \mathbf{p}_i)|^2}{|\mathbf{p}_i|_{\sigma_{\text{tot}}}(\mathbf{p}_i)}. \quad (66)$$

Arriving at this equation required a certain amount of heuristic argumentation. It should be emphasized that this expression was already used in [6], where it was shown to yield a localization rate for collisional decoherence that is equal to a wave packet calculation similar to the one in Sect. V.

If we accept (66) the evaluation of the complex rate density m_{in} can be done in a rather straightforward fashion. Using the unrestricted rate operator Γ_0 and the modified T'_0 instead of T_0 , the complex rate density from (40) takes the form

$$m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}) = \Gamma_0^{1/2}(\mathbf{p}_i + \mathbf{q}) \Gamma_0^{1/2}(\mathbf{p}_i - \mathbf{q}) \xi(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}) \quad (67)$$

with the formal expression

$$\xi(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}) = \frac{(2\pi\hbar)^3}{|\Omega|} \langle \mathbf{p}_f + \mathbf{q} | \mathcal{T}'_0 | \mathbf{p}_i + \mathbf{q} \rangle \times \langle \mathbf{p}_f - \mathbf{q} | \mathcal{T}'_0 | \mathbf{p}_i - \mathbf{q} \rangle^*. \quad (68)$$

The latter can be evaluated by means of Eq. (66). For $\mathbf{q} = 0$ we have immediately

$$\xi(\mathbf{p}_f, \mathbf{p}_i; 0) = \delta\left(\frac{\mathbf{p}_f^2 - \mathbf{p}_i^2}{2}\right) \frac{|f(\mathbf{p}_f, \mathbf{p}_i)|^2}{\sigma_{\text{tot}}(\mathbf{p}_i) |\mathbf{p}_i|}, \quad (69)$$

while for $\mathbf{q} \neq 0$ an extension of the rule (66) to different pairs of incoming and outgoing relative momenta is required. It can be constructed by formally taking the square root of (66). Insertion into (68) brings about the square root of a product of two energy conserving δ -functions with arguments $\frac{\mathbf{p}_f^2 - \mathbf{p}_i^2}{2} \pm (\mathbf{p}_f - \mathbf{p}_i) \cdot \mathbf{q}$. Like with the delta-functions in Sect. V B, this product implies that the parallel component \mathbf{q}_{\parallel} of the momentum separation must be zero, thus restricting a \mathbf{q} -integration to the plane perpendicular to the momentum change $\mathbf{p}_f - \mathbf{p}_i$,

$$\xi(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}) = \begin{cases} \xi(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}_{\perp}) & \text{if } \mathbf{q}_{\parallel} = 0 \\ 0 & \text{otherwise.} \end{cases} \quad (70)$$

The formal square root of the product of delta functions then reduces to a single proper Dirac function $\delta\left(\left(\mathbf{p}_f^2 - \mathbf{p}_i^2\right)/2\right)$, and we obtain, as the natural generalization of (66),

$$\xi(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}_{\perp}) = \delta\left(\frac{\mathbf{p}_f^2 - \mathbf{p}_i^2}{2}\right) \frac{f(\mathbf{p}_f + \mathbf{q}_{\perp}, \mathbf{p}_i + \mathbf{q}_{\perp})}{\sqrt{\sigma_{\text{tot}}(\mathbf{p}_i + \mathbf{q}_{\perp})} |\mathbf{p}_i + \mathbf{q}_{\perp}|} \times \frac{f^*(\mathbf{p}_f - \mathbf{q}_{\perp}, \mathbf{p}_i - \mathbf{q}_{\perp})}{\sqrt{\sigma_{\text{tot}}(\mathbf{p}_i - \mathbf{q}_{\perp})} |\mathbf{p}_i - \mathbf{q}_{\perp}|}. \quad (71)$$

Inserting this expression into (67), together with rates determined by (44), one arrives directly at the complex rate density m_{in} given by Eqs. (41), (42).

We emphasize again that, compared to the microscopic phase space description in the preceding section, the line of reasoning is here quite different, and indeed more heuristic. The fact that the two lines of argument yield identical results indicates that their specific assumptions do reflect the underlying physics.

VII. THE GAS INDUCED ENERGY SHIFT

We now turn to the second part of the master equation, given by the superoperator \mathcal{R} defined in Eq. (5). This term describes the coherent modification of the tracer particle dynamics due to the presence of the gas. As with the incoherent part \mathcal{L} given in (4), a naive evaluation would take the expressions (11) and (13) for the rate and scattering operators at face value, and would thus

yield an ill-defined normalization involving a $\delta(0)/|\Omega|$ term. The correct normalization will be obtained in this section by implementing the appropriate restriction to the incoming states in the same way as in Sect. V.

It should be noted that the effect of the energy shift described by \mathcal{R} can usually be neglected when the incoherent effects of the master equation play a role so that \mathcal{L} dominates the dynamics. However, one can set up atom interferometer experiments where one beam interacts with a gas filled region such that only those atoms contribute to the detected signal which did not change their momentum by a collision. In this case, the effect can be measured as a gas-induced phase shift, and it is usually accounted for by attributing a refractive index to the gas [27, 28, 29, 30, 31].

Before starting the calculation, let us note that in Ref. [9] a slightly different term was given for the coherent modification, namely $\mathcal{R}'\rho = i \text{Tr}_{\text{gas}}([\text{Re}(\mathcal{T}), \Gamma^{1/2} [\rho \otimes \rho_{\text{gas}}] \Gamma^{1/2}])$. It differs from (5) in the location of one of the $\Gamma^{1/2}$ operators. In fact, the two superoperators \mathcal{R} and \mathcal{R}' yield the same gas induced energy shift when applied to the immobile system discussed in [9]. For the present case of a tracer particle, \mathcal{R}' has the disadvantage of introducing a weak dependence on P/P' which would need to be removed as an additional approximation. It therefore seems more natural to start from the form (5) right away, which is manifestly unitary.

The calculational procedure can be carried out in complete analogy to the reasoning in Sect. V. Inserting the stationary state (8) into the expression (5) for $\mathcal{R}\rho$ yields immediately the coherent modification of the evolution due to the presence of the gas. In momentum representation it takes the form of Eq. (29) with the energy shifts given by

$$E_n(\mathbf{P}) = -\hbar \frac{(2\pi\hbar)^3}{|\Omega|} \int d\mathbf{p}_0 \mu(\mathbf{p}_0) \times \langle \text{rel}(\mathbf{p}_0, \mathbf{P}) | \Gamma_0^{1/2} \text{Re}(\mathcal{T}_0) \Gamma_0^{1/2} | \text{rel}(\mathbf{p}_0, \mathbf{P}) \rangle. \quad (72)$$

We can again switch to the center-of-mass frame by introducing the relative momentum

$$\mathbf{p}_n = \text{rel}(\mathbf{p}_0, \mathbf{P}) \quad (73)$$

as a function of \mathbf{p}_0 . This way the energy shifts take the form of an average over the gas momentum distribution function μ ,

$$E_n(\mathbf{P}) = \int d\mathbf{p}_0 \mu(\mathbf{p}_0) e_n(\mathbf{p}_n). \quad (74)$$

Like in the incoherent case, the function to be averaged can again be written as an expectation value with respect to a normalized momentum state of the relative motion $\rho_{\mathbf{p}_n} = |\mathbf{p}_n\rangle\rangle\langle\langle\mathbf{p}_n|$. The function has the unit of an energy,

$$e_n(\mathbf{p}_n) = -\hbar \text{Tr} \left(\Gamma_0^{1/2} \text{Re}(\mathcal{T}_0) \Gamma_0^{1/2} \rho_{\mathbf{p}_n} \right). \quad (75)$$

When evaluating the expectation value, the restriction to incoming wave packets can again be implemented by replacing $\rho_{\mathbf{p}_n}$ with its restricted version $\rho'_{\mathbf{p}_n}$. It is given by Eq. (55) with \mathbf{p}_i replaced by \mathbf{p}_n , see Fig. 2. One thus obtains

$$e_n(\mathbf{p}_n) = -\frac{1}{2\pi} \int d\mathbf{w} \int_{\Lambda_{\mathbf{p}_n}} \frac{d\mathbf{x}_{\parallel\mathbf{p}_n}}{|\Lambda_{\mathbf{p}_n}|} \int_{\Sigma_{\mathbf{p}_n}} \frac{d\mathbf{x}_{\perp\mathbf{p}_n}}{|\Sigma_{\mathbf{p}_n}|} \\ \times \exp\left(i\frac{\mathbf{x} \cdot \mathbf{w}}{\hbar}\right) \Gamma_0^{1/2}\left(\mathbf{p}_n + \frac{\mathbf{w}}{2}\right) \Gamma_0^{1/2}\left(\mathbf{p}_n - \frac{\mathbf{w}}{2}\right) \\ \times \delta(\mathbf{p}_n \cdot \mathbf{w}) \operatorname{Re}\left[f\left(\mathbf{p}_n + \frac{\mathbf{w}}{2}, \mathbf{p}_n - \frac{\mathbf{w}}{2}\right)\right].$$

Like in Sect. V, we identify the cylinder base area with the scattering cross section, $|\Sigma_{\mathbf{p}_n}| = \sigma(\mathbf{p}_n)$, and we note that the delta-function removes the component of \mathbf{w} which is parallel to \mathbf{p}_n , so that the dependence on $\mathbf{x}_{\parallel\mathbf{p}_n}$ vanishes in the integrand,

$$e_n(\mathbf{p}_n) = -2\pi\hbar^2 \frac{n_{\text{gas}}}{m_*} \int d\mathbf{w} \delta\left(\frac{\mathbf{p}_n \cdot \mathbf{w}}{p_n}\right) \\ \times \int_{\Sigma_{\mathbf{p}_n}} \frac{d\mathbf{x}_{\perp\mathbf{p}_n}}{(2\pi\hbar)^2} \exp\left(i\frac{\mathbf{x}_{\perp\mathbf{p}_n} \cdot \mathbf{w}_{\perp\mathbf{p}_n}}{\hbar}\right) \\ \times \int_{\Lambda_{\mathbf{p}_n}} \frac{d\mathbf{x}_{\parallel\mathbf{p}_n}}{|\Lambda_{\mathbf{p}_n}|} \operatorname{Re}\left[f\left(\mathbf{p}_n + \frac{\mathbf{w}}{2}, \mathbf{p}_n - \frac{\mathbf{w}}{2}\right)\right] \\ \times \frac{\sqrt{|\mathbf{p}_n + \frac{\mathbf{w}}{2}| |\mathbf{p}_n - \frac{\mathbf{w}}{2}|}}{p_n} \\ \times \frac{\sqrt{\sigma(\mathbf{p}_n + \frac{\mathbf{w}}{2}) \sigma(\mathbf{p}_n - \frac{\mathbf{w}}{2})}}{\sigma(\mathbf{p}_n)}.$$

Carrying out the $\mathbf{x}_{\parallel\mathbf{p}_n}$ -integration, $\int_{\Lambda_{\mathbf{p}_n}} d\mathbf{x}_{\parallel\mathbf{p}_n} = |\Lambda_{\mathbf{p}_n}|$, one observes that the remaining $\mathbf{x}_{\perp\mathbf{p}_n}$ -integration yields an approximate two-dimensional delta-function in $\mathbf{w}_{\perp\mathbf{p}_n}$. Combined with the delta function in $\mathbf{p}_n \cdot \mathbf{w}/p_n = w_{\parallel\mathbf{p}_n}$ this gives a three-dimensional $\delta(\mathbf{w})$, which permits to do the \mathbf{w} -integration. One thus obtains

$$e_n(\mathbf{p}_n) = -2\pi\hbar^2 \frac{n_{\text{gas}}}{m_*} \operatorname{Re}[f(\mathbf{p}_n, \mathbf{p}_n)]. \quad (76)$$

It shows that the energy shift is essentially determined by the real part of the forward scattering amplitude, a fact that is well-known in the field of neutron and atom optics. Its effect is often expressed by introducing an index of refraction n_1 , as discussed in Sect. IX E.

VIII. OPERATOR REPRESENTATION OF THE QUANTUM LINEAR BOLTZMANN EQUATION

So far, the derivation of the master equation was discussed in the momentum representation. Let us now turn to the question how to obtain the quantum linear Boltzmann equation in a representation-independent form. The result will then immediately prove the complete positivity and the translational covariance of the dynamical map defined by the master equation.

The calculations in Sects. V and VI both indicate that m_{in} , the rate function in the center of mass frame, is given by Eq. (42). The complex rate M_{in} , which determines the incoherent evolution in momentum representation according to (17), is then obtained by averaging m_{in} with the gas momentum distribution function μ . Specifically, Eq. (39) tells that $M_{\text{in}}(\mathbf{P}, \mathbf{P}'; \mathbf{Q}) = \int d\mathbf{p}_0 \mu(\mathbf{p}_0) m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q})$ with the relative momenta \mathbf{p}_f , \mathbf{p}_i , and \mathbf{q} defined in (33)-(35). However, the resulting expression is not of the factorized form (27) needed below when stating the master equation in its operator representation.

To arrive at (27) we first change the integration variable from \mathbf{p}_0 to \mathbf{p}_i . Moreover, the μ distribution can be split symmetrically into a product of square roots, $\mu(\mathbf{p}_0) = \mu^{1/2}(\mathbf{p}_0) \mu^{1/2}(\mathbf{p}_0)$, since \mathbf{p}_0 can be equally expressed as $\mathbf{p}_i + (\mathbf{p}_f + \mathbf{P})m/M + \mathbf{q}m/m_*$ or as $\mathbf{p}_i + (\mathbf{p}_f + \mathbf{P}')m/M - \mathbf{q}m/m_*$, see (33)-(35). Noting $|\det(\partial\mathbf{p}_0/\partial\mathbf{p}_i)| = m^3/m_*^3$ we have

$$M_{\text{in}}(\mathbf{P}, \mathbf{P}'; \mathbf{Q}) \\ = \left(\frac{m}{m_*}\right)^3 \int d\mathbf{p}_i \mu^{1/2}\left(\mathbf{p}_i + \frac{m}{M}(\mathbf{p}_f + \mathbf{P}) + \frac{m}{m_*}\mathbf{q}_{\perp}\right) \\ \times \mu^{1/2}\left(\mathbf{p}_i + \frac{m}{M}(\mathbf{p}_f + \mathbf{P}') - \frac{m}{m_*}\mathbf{q}_{\perp}\right) \\ \times m_{\text{in}}(\mathbf{p}_f, \mathbf{p}_i; \mathbf{q}_{\perp}),$$

where we replaced \mathbf{q} by \mathbf{q}_{\perp} in the arguments of $\mu^{1/2}$, in accordance with Eq. (48). Having implemented the property (41) of the generalized function m_{in} , we can now insert its explicit form (42), which introduces the scattering amplitudes and an energy conserving delta-function,

$$M_{\text{in}}(\mathbf{P}, \mathbf{P}'; \mathbf{Q}) \\ = \left(\frac{m}{m_*}\right)^3 \int d\mathbf{p}_i \mu^{1/2}\left(\mathbf{p}_i + \frac{m}{M}(\mathbf{p}_f + \mathbf{P}) + \frac{m}{m_*}\mathbf{q}_{\perp}\right) \\ \times \mu^{1/2}\left(\mathbf{p}_i + \frac{m}{M}(\mathbf{p}_f + \mathbf{P}') - \frac{m}{m_*}\mathbf{q}_{\perp}\right) \delta\left(\frac{\mathbf{p}_f^2 - \mathbf{p}_i^2}{2}\right) \\ \times \frac{n_{\text{gas}}}{m_*} f(\mathbf{p}_f + \mathbf{q}_{\perp}, \mathbf{p}_i + \mathbf{q}_{\perp}) f^*(\mathbf{p}_f - \mathbf{q}_{\perp}, \mathbf{p}_i - \mathbf{q}_{\perp}). \quad (77)$$

From here it is a small step to arrive at the explicit expression given in Eq. (24). In order to obtain a factorized expression we rather perform another change of variables,

$$\mathbf{p}_i \rightarrow \mathbf{p} = \frac{m}{m_*}\mathbf{p}_i + \frac{m}{M}\frac{\mathbf{P}_{\perp}\mathbf{Q} + \mathbf{P}'_{\perp}\mathbf{Q}}{2} - \frac{m}{m_*}\frac{\mathbf{Q}}{2}.$$

Due to its dependence on the transverse \mathbf{P} and \mathbf{P}' components this transformation has the remarkable effect of producing an integrand which is a product of \mathbf{P} - and

\mathbf{P}' -dependent factors:

$$\begin{aligned}
M_{\text{in}}(\mathbf{P}, \mathbf{P}'; \mathbf{Q}) &= \frac{n_{\text{gas}}}{m_*} \int d\mathbf{p} \mu^{1/2} \left(\mathbf{p} + \frac{m}{M} \mathbf{P}_{\parallel} + \left(1 - \frac{m}{M}\right) \frac{\mathbf{Q}}{2} \right) \\
&\times \mu^{1/2} \left(\mathbf{p} + \frac{m}{M} \mathbf{P}'_{\parallel} + \left(1 - \frac{m}{M}\right) \frac{\mathbf{Q}}{2} \right) \delta\left(\frac{m_*}{m} \mathbf{p} \cdot \mathbf{Q}\right) \\
&\times f\left(\text{rel}(\mathbf{p}, \mathbf{P}_{\perp}) - \frac{\mathbf{Q}}{2}, \text{rel}(\mathbf{p}, \mathbf{P}_{\perp}) + \frac{\mathbf{Q}}{2}\right) \\
&\times f^*\left(\text{rel}(\mathbf{p}, \mathbf{P}'_{\perp}) - \frac{\mathbf{Q}}{2}, \text{rel}(\mathbf{p}, \mathbf{P}'_{\perp}) + \frac{\mathbf{Q}}{2}\right) \\
&= \int d\mathbf{p} \delta\left(\frac{\mathbf{p} \cdot \mathbf{Q}}{Q}\right) L(\mathbf{p}, \mathbf{P} - \mathbf{Q}; \mathbf{Q}) L^*(\mathbf{p}, \mathbf{P}' - \mathbf{Q}; \mathbf{Q}).
\end{aligned} \tag{78}$$

The second equality, which brings about the functions $L(\mathbf{p}, \mathbf{P}; \mathbf{Q})$ defined in Eq. (28), emphasizes the factorization. Observing that the delta function restricts the \mathbf{p} -integration to the plane $\mathbf{Q}^{\perp} = \{\mathbf{p} \in \mathbb{R}^3 : \mathbf{p} \cdot \mathbf{Q} = 0\}$ perpendicular to \mathbf{Q} finally leads to the expression announced in Eq. (27), since for any function $g(\mathbf{p})$

$$\int d\mathbf{p} \delta\left(\frac{\mathbf{p} \cdot \mathbf{Q}}{Q}\right) g(\mathbf{p}) = \int_{\mathbf{Q}^{\perp}} d\mathbf{p} g(\mathbf{p}). \tag{79}$$

The function L from Eq. (28) is clearly well-suited to characterize the master equation, since it contains all the details of the collisional interaction with the gas. It comprises the elastic scattering amplitude $f(\mathbf{p}_f, \mathbf{p}_i)$ defined by the two-body interaction, the mass M of the tracer particle, the momentum distribution function $\mu(\mathbf{p})$ of the gas, its mass m and number density n_{gas} . Unsurprisingly, the function L plays a central role for the operator representation of the master equation as well. It permits to define a family of jump operators acting in the Hilbert space of the tracer particle,

$$\mathcal{L}_{\mathbf{Q}, \mathbf{P}} = e^{i\mathbf{X} \cdot \mathbf{Q}/\hbar} L(\mathbf{p}, \mathbf{P}; \mathbf{Q}), \tag{80}$$

where \mathbf{X} and \mathbf{P} are the corresponding position and momentum operators (and the function L is given in Eq. (28)). The first factor effects a momentum exchange by \mathbf{Q} , since $\exp(i\mathbf{X} \cdot \mathbf{Q}/\hbar) |\mathbf{P}\rangle = |\mathbf{P} + \mathbf{Q}\rangle$, while the appearance of \mathbf{P} in the second factor renders the function L operator valued. This implies that both the scattering amplitude and the momentum distribution function attain an operator character in (28), which is possible because the \mathbf{P} -dependence of L will be analytic for any physically reasonable interaction potential.

With the jump operators (80) at hand it is straightforward to construct the superoperator \mathcal{L} , whose momentum representation is given by Eq. (17) with M_{in} from (27),

$$\begin{aligned}
\mathcal{L}\rho &= \int d\mathbf{Q} \int_{\mathbf{Q}^{\perp}} d\mathbf{p} \left\{ \mathcal{L}_{\mathbf{Q}, \mathbf{P}} \rho \mathcal{L}_{\mathbf{Q}, \mathbf{P}}^{\dagger} - \frac{1}{2} \rho \mathcal{L}_{\mathbf{Q}, \mathbf{P}}^{\dagger} \mathcal{L}_{\mathbf{Q}, \mathbf{P}} \right. \\
&\quad \left. - \frac{1}{2} \mathcal{L}_{\mathbf{Q}, \mathbf{P}}^{\dagger} \mathcal{L}_{\mathbf{Q}, \mathbf{P}} \rho \right\}.
\end{aligned} \tag{81}$$

This is the equation given in Ref. [10] (up to a trivial change of notation).

It is reassuring to observe that the form of the generator (81) is in accordance with the most general structure of a translation-invariant and completely positive master equation as characterized by Holevo [32], see [33, 34] for a discussion. However, the summation in Ref. [32] is here replaced by the \mathbf{p} -integration over the plane \mathbf{Q}^{\perp} in (81).

A further consistency requirement is based on the transformation to a moving frame of reference. Denoting the velocity boost by \mathbf{V} , the transformed state of the tracer particle is given by

$$\rho_{\mathbf{V}} = e^{i\mathbf{X} \cdot M\mathbf{V}/\hbar} \rho e^{-i\mathbf{X} \cdot M\mathbf{V}/\hbar},$$

and the incoherent evolution in the new frame of reference $\mathcal{L}_{\mathbf{V}}$ is thus related to \mathcal{L} by

$$\mathcal{L}_{\mathbf{V}}[\cdot] = e^{i\mathbf{X} \cdot M\mathbf{V}/\hbar} \mathcal{L} \left[e^{-i\mathbf{X} \cdot M\mathbf{V}/\hbar} \cdot e^{i\mathbf{X} \cdot M\mathbf{V}/\hbar} \right] e^{-i\mathbf{X} \cdot M\mathbf{V}/\hbar} \tag{82}$$

However, the same super-operator must be obtained if we *actively* shift the momentum distribution $\mu(\mathbf{p})$ of the background gas, by setting $\mu_{\mathbf{V}}(\mathbf{p}) = \mu(\mathbf{p} - m\mathbf{V})$ in the function L defining the jump operators (80). The reason why this transformation of the gas motion must have the same effect as (82) is that the interaction between the tracer particle and the gas depends only on their relative motion. Indeed, the functions L and $L_{\mathbf{V}}$, based on the gas distributions μ and $\mu_{\mathbf{V}}$ in (28), are related by $L(\mathbf{p}, \mathbf{P} - m\mathbf{V}; \mathbf{Q}) = L_{\mathbf{V}}(\mathbf{p} + m\mathbf{V}_{\perp \mathbf{Q}}, \mathbf{P}; \mathbf{Q})$. Noting also that a change of the integration variable $\mathbf{p} \rightarrow \mathbf{p}'_{\perp} = \mathbf{p} + m\mathbf{V}_{\perp \mathbf{Q}}$ in (81) is possible, since it leaves the plane \mathbf{Q}^{\perp} invariant, one easily proves the equivalence of the coordinate transformation and the shift of the momentum distribution.

As a final step, let us also incorporate the coherent modification of the tracer dynamics as discussed in Sect. VII. The energy shift operator

$$\mathbf{H}_{\text{n}} = E_{\text{n}}(\mathbf{P}) \tag{83}$$

is given by the operator-valued version of Eq. (30). It permits to write the coherent modification part of the master equation (29) as $\mathcal{R}\rho = (i\hbar)^{-1} [\mathbf{H}_{\text{n}}, \rho]$. This super-operator has the same invariance and transformation properties as discussed above in the case of \mathcal{L} . In particular, its transformation to a moving frame of reference analogous to (82) is equally obtained by replacing μ with $\mu_{\mathbf{V}}$ in (30).

To summarize this section we include the free motion Hamiltonian $\mathbf{H} = \mathbf{P}^2/2M$, thus writing the complete quantum linear Boltzmann equation (3) in the representation-independent form

$$\begin{aligned}
\partial_t \rho &= \frac{1}{i\hbar} \left[\frac{\mathbf{P}^2}{2M} + \mathbf{H}_{\text{n}}, \rho \right] + \frac{1}{2} \int d\mathbf{Q} \int_{\mathbf{Q}^{\perp}} d\mathbf{p} \left\{ \left[\mathcal{L}_{\mathbf{Q}, \mathbf{P}}, \rho \mathcal{L}_{\mathbf{Q}, \mathbf{P}}^{\dagger} \right] \right. \\
&\quad \left. + \left[\mathcal{L}_{\mathbf{Q}, \mathbf{P}} \rho, \mathcal{L}_{\mathbf{Q}, \mathbf{P}}^{\dagger} \right] \right\}.
\end{aligned} \tag{84}$$

IX. LIMITING FORMS

As an important cross-check of the QLBE derived above, let us now see whether taking suitable limits reduces its form to that of previously established equations.

A. Classical linear Boltzmann equation

The most obvious limiting motion is that of a classical particle. If all off-diagonal elements vanish in a motional state, $\langle \mathbf{P} | \rho | \mathbf{P}' \rangle = 0$, it is characterized by the diagonal momentum distribution $f_p(\mathbf{P}) = \langle \mathbf{P} | \rho | \mathbf{P} \rangle$ alone, and insofar it is indistinguishable from a classical state. One expects that the motion of the diagonal elements predicted by (81) is equal to the one described by the classical linear Boltzmann equation.

As follows from the discussion in Sect. III, the QLBE implies that the diagonal elements $f_p(\mathbf{P})$ satisfy

$$\partial_t^{\text{coll}} f_p(\mathbf{P}) = \int d\mathbf{Q} M_{\text{in}}^{\text{cl}}(\mathbf{P}; \mathbf{Q}) f_p(\mathbf{P} - \mathbf{Q}) - M_{\text{out}}^{\text{cl}}(\mathbf{P}) f_p(\mathbf{P}), \quad (85)$$

with the rates $M_{\text{out}}^{\text{cl}}(\mathbf{P})$ and $M_{\text{in}}^{\text{cl}}(\mathbf{P}; \mathbf{Q})$ given by Eqs. (20) and (22). The notation ∂_t^{coll} indicates that we focus here only on the differential change in time which is due to the collision part \mathcal{L} of the master equation.

This equation should be compared to the classical linear Boltzmann equation [2] for the momentum distribution function $f_p^{\text{cl}}(\mathbf{P})$. The traditional form of the collision integral reads, in our notation,

$$\begin{aligned} \partial_t^{\text{coll}} f_p^{\text{cl}}(\mathbf{P}) &= n_{\text{gas}} \int d\mathbf{p} d\mathbf{n} \frac{|\text{rel}(\mathbf{p}, \mathbf{P})|}{m_*} \\ &\times \sigma(|\text{rel}(\mathbf{p}, \mathbf{P})|, \mathbf{n}, \text{rel}(\mathbf{p}, \mathbf{P})) \\ &\times \{ \mu(\mathbf{p}') f_p^{\text{cl}}(\mathbf{P}') - \mu(\mathbf{p}) f_p^{\text{cl}}(\mathbf{P}) \}, \end{aligned} \quad (86)$$

where \mathbf{n} is the unit vector of an angular integration with $d\mathbf{n}$ the associated element of solid angle. The values of \mathbf{P}' and \mathbf{p}' are determined by momentum conservation, granting in particular $|\text{rel}(\mathbf{p}', \mathbf{P}')| = |\text{rel}(\mathbf{p}, \mathbf{P})|$. Using the PT-invariance of the differential cross section, $\sigma(\mathbf{p}_f, \mathbf{p}_i) = \sigma(\mathbf{p}_i, \mathbf{p}_f)$, the classical linear Boltzmann equation can thus be rewritten in the explicit form

$$\begin{aligned} \partial_t^{\text{coll}} f_p^{\text{cl}}(\mathbf{P}) &= \frac{n_{\text{gas}}}{m_*} \int d\mathbf{p} d\mathbf{n}_i |\text{rel}(\mathbf{p}, \mathbf{P})| \\ &\times \mu(\mathbf{p} - \text{rel}(\mathbf{p}, \mathbf{P}) + |\text{rel}(\mathbf{p}, \mathbf{P})| \mathbf{n}_i) \\ &\times \sigma(\text{rel}(\mathbf{p}, \mathbf{P}), |\text{rel}(\mathbf{p}, \mathbf{P})| \mathbf{n}_i) \\ &\times f_p^{\text{cl}}(\mathbf{P} + \text{rel}(\mathbf{p}, \mathbf{P}) - |\text{rel}(\mathbf{p}, \mathbf{P})| \mathbf{n}_i) \\ &- f_p^{\text{cl}}(\mathbf{P}) \frac{n_{\text{gas}}}{m_*} \int d\mathbf{p} d\mathbf{n}_f |\text{rel}(\mathbf{p}, \mathbf{P})| \\ &\times \mu(\mathbf{p}) \sigma(|\text{rel}(\mathbf{p}, \mathbf{P})| \mathbf{n}_f, \text{rel}(\mathbf{p}, \mathbf{P})). \end{aligned} \quad (87)$$

The angular integrations can be converted into three-dimensional integrals with a delta function. Noting

$$\begin{aligned} &|\text{rel}(\mathbf{p}, \mathbf{P})| \delta(|\mathbf{p}_{i,f}| - |\text{rel}(\mathbf{p}, \mathbf{P})|) \\ &= p_{i,f}^2 \delta\left(\frac{|\mathbf{p}_{i,f}|^2 - |\text{rel}(\mathbf{p}, \mathbf{P})|^2}{2}\right) \end{aligned}$$

one arrives, after the substitutions $\mathbf{p}_{i,f} \rightarrow \mathbf{P}_{i,f} = \mathbf{P} + \text{rel}(\mathbf{p}, \mathbf{P}) - \mathbf{p}_{i,f}$, at the form

$$\begin{aligned} \partial_t^{\text{coll}} f_p^{\text{cl}}(\mathbf{P}) &= \int d\mathbf{P}_i M^{\text{cl}}(\mathbf{P}_i \rightarrow \mathbf{P}) f_p^{\text{cl}}(\mathbf{P}_i) \\ &- f_p^{\text{cl}}(\mathbf{P}) \int d\mathbf{P}_f M^{\text{cl}}(\mathbf{P} \rightarrow \mathbf{P}_f) \end{aligned} \quad (88)$$

with the classical rate density for the change of the tracer particle momentum from \mathbf{P}_i to \mathbf{P}_f given by

$$\begin{aligned} M^{\text{cl}}(\mathbf{P}_i \rightarrow \mathbf{P}_f) &= \frac{n_{\text{gas}}}{m_*} \int d\mathbf{p}_0 \mu(\mathbf{p}_0) \sigma(\text{rel}(\mathbf{p}_0, \mathbf{P}_i) + \mathbf{P}_i - \mathbf{P}_f, \text{rel}(\mathbf{p}_0, \mathbf{P}_i)) \\ &\times \delta\left(\frac{|\text{rel}(\mathbf{p}_0, \mathbf{P}_i) + \mathbf{P}_i - \mathbf{P}_f|^2 - |\text{rel}(\mathbf{p}_0, \mathbf{P}_i)|^2}{2}\right). \end{aligned} \quad (89)$$

It is now easy to see that the form (88) of the classical linear Boltzmann equation is indeed identical to the diagonal part (85) of the QLBE, with $M_{\text{out}}^{\text{cl}}(\mathbf{P})$ and $M_{\text{in}}^{\text{cl}}(\mathbf{P}; \mathbf{Q})$ given by Eqs. (20) and (22).

B. Pure collisional decoherence

Another possible effect of the gas on a quantum tracer particle, and in a sense the other extreme compared to the classical dynamics on the diagonal, is the appearance of *pure* collisional decoherence. It follows from the QLBE (81) in the limit where the mass M of the tracer particle is much larger than the mass m of the gas molecules, so that there is no energy exchange during a collision. Taking m/M to zero simplifies the function (28) characterizing the jump operators in (80), and renders it independent of \mathbf{P} ,

$$\begin{aligned} L(\mathbf{p}, \mathbf{P}; \mathbf{Q}) &\xrightarrow{\frac{m}{M} \rightarrow 0} \sqrt{\frac{n_{\text{gas}}}{Qm}} \mu\left(\mathbf{p}_{\perp Q} + \frac{\mathbf{Q}}{2}\right)^{1/2} \\ &\times f\left(\mathbf{p}_{\perp Q} - \frac{\mathbf{Q}}{2}, \mathbf{p}_{\perp Q} + \frac{\mathbf{Q}}{2}\right). \end{aligned} \quad (90)$$

It follows that the generator of the incoherent evolution (81) reduces to the form⁴

$$\mathcal{L}\rho \xrightarrow{\frac{m}{M} \rightarrow 0} \frac{n_{\text{gas}}}{m} \int d\mathbf{p}_i d\mathbf{p}_f \mu(\mathbf{p}_i) \delta\left(\frac{\mathbf{p}_f^2 - \mathbf{p}_i^2}{2}\right) \sigma(\mathbf{p}_f, \mathbf{p}_i) \times \left\{ e^{i\mathbf{X} \cdot (\mathbf{p}_i - \mathbf{p}_f)/\hbar} \rho e^{-i\mathbf{X} \cdot (\mathbf{p}_i - \mathbf{p}_f)/\hbar} - \rho \right\}. \quad (91)$$

This is the master equation of pure collisional decoherence discussed by Gallis and Fleming [5] and derived in its final form in Ref. [6]. It describes an exponential decay of the off-diagonal elements in position representation,

$$\langle \mathbf{X} | \mathcal{L}\rho | \mathbf{X}' \rangle \xrightarrow{\frac{m}{M} \rightarrow 0} -F(\mathbf{X} - \mathbf{X}') \langle \mathbf{X} | \rho | \mathbf{X}' \rangle, \quad (92)$$

with a localization rate given by

$$F(\mathbf{R} - \mathbf{R}') = \frac{n_{\text{gas}}}{m} \int d\mathbf{p}_i d\mathbf{p}_f \mu(\mathbf{p}_i) \delta\left(\frac{\mathbf{p}_i^2 - \mathbf{p}_f^2}{2}\right) \times \sigma(\mathbf{p}_f, \mathbf{p}_i) \left\{ 1 - e^{i(\mathbf{R} - \mathbf{R}') \cdot (\mathbf{p}_i - \mathbf{p}_f)/\hbar} \right\}. \quad (93)$$

This loss of coherence in the position basis can be attributed to the amount of position information (or ‘which path’ information) gained by the colliding gas. Recently, it has been observed that interfering fullerene molecules display a reduction of interference visibility in agreement with this equation [7, 35, 36].

C. Specialization to the Maxwell-Boltzmann distribution

So far, we kept the momentum distribution μ of the gas molecules unspecified. This served to highlight the generality of the equations and it permitted, at the end of Sect. VIII, to discuss the implications of a transformation of the momentum distribution. However, the most important choice is of course that of a Maxwell gas, characterized by a temperature $T = 1/\beta k_B$. The remaining discussions of limiting forms in this section will be done with the corresponding Maxwell-Boltzmann distribution,

$$\mu_\beta(\mathbf{p}) = \frac{1}{\pi^{3/2} p_\beta^3} \exp\left(-\frac{\mathbf{p}^2}{p_\beta^2}\right), \quad (94)$$

where $p_\beta = \sqrt{2m/\beta}$ is the most probable momentum. We note that the statistical operator of the gas then takes the form

$$\rho_{\text{gas}}^\beta = \frac{\lambda_{\text{th}}^3}{|\Omega|} \mathbf{l}_\Omega \exp\left(-\beta \frac{\mathbf{p}^2}{2m}\right) \mathbf{l}_\Omega \quad (95)$$

with $\lambda_{\text{th}} = \sqrt{2\pi\hbar^2\beta/m}$ the thermal de Broglie wave length and \mathbf{l}_Ω the projectors to the normalization region, which are known from (6).

D. Weak coupling result

A first limiting form of the QLBE that was obtained for the Maxwell-Boltzmann distribution is the weak coupling result by one of us [11, 12, 13]. Its derivation differs strongly from the approach of the present article, using the van Hove expression to relate the dynamic structure factor of the gas to the differential cross section in the laboratory frame.

It can be regained from the present QLBE by replacing the exact scattering amplitude f in (28) by its Born approximation f_B , which is proportional to the Fourier transform of the interaction potential,

$$f_B(\mathbf{p}_f, \mathbf{p}_i) = -4\pi^2 \hbar m_* \langle \mathbf{p}_f | V(\mathbf{x}) | \mathbf{p}_i \rangle \quad (96)$$

$$= -\frac{m_*}{2\pi\hbar^2} \int d\mathbf{x} V(\mathbf{x}) \exp\left(-i\frac{(\mathbf{p}_f - \mathbf{p}_i) \cdot \mathbf{x}}{\hbar}\right).$$

Importantly, the Born approximation depends only on the momentum transfer $\mathbf{p}_f - \mathbf{p}_i$, but not on the energy in the relative motion. Even though f_B violates the unitarity relation expressed by the optical theorem, it can be used to approximate the scattering amplitude if the energy of the relative motion is much larger than the interaction energy.

Inserting the Born approximation (96) into the function (28) defining the jump operators $\mathbf{L}_{\mathbf{Q}, \mathbf{P}} = e^{i\mathbf{X} \cdot \mathbf{Q}/\hbar} L(\mathbf{p}, \mathbf{P}; \mathbf{Q})$ from Sect. VIII, one notes that the \mathbf{P} -dependence *drops out* in the scattering amplitude. As a result, the Born approximation of the function (28) can be written as

$$L_B(\mathbf{p}, \mathbf{P}; \mathbf{Q}) = \left[\frac{n_{\text{gas}}}{m_*^2}\right]^{1/2} f_B(-\mathbf{Q}) \sqrt{S(\mathbf{Q}, \mathbf{P})} \times \frac{1}{\sqrt{\pi^{1/2} p_\beta}} \exp\left(-\frac{\mathbf{p}_\perp^2 \mathbf{Q}}{2p_\beta^2}\right), \quad (97)$$

where $S(\mathbf{Q}, \mathbf{P})$ is the dynamic structure factor of the Maxwell gas [37],

$$S(\mathbf{Q}, \mathbf{P}) = \sqrt{\frac{\beta m}{2\pi}} \frac{1}{Q} \exp\left(-\beta \frac{\left((1 + \frac{m}{M})Q^2 + 2\frac{m}{M}\mathbf{P} \cdot \mathbf{Q}\right)^2}{8mQ^2}\right). \quad (98)$$

Since the \mathbf{p} -dependence in (97) appears just as a factor, one can carry out the \mathbf{Q}^\perp -integration in the operator representation (81) of the master equation. The weak coupling approximation of the QLBE thus reduces to the form

$$\mathcal{L}^B \rho = \int d\mathbf{Q} \left\{ \tilde{\mathbf{L}}_{\mathbf{Q}} \rho \tilde{\mathbf{L}}_{\mathbf{Q}}^\dagger - \frac{1}{2} \tilde{\mathbf{L}}_{\mathbf{Q}}^\dagger \tilde{\mathbf{L}}_{\mathbf{Q}} - \frac{1}{2} \tilde{\mathbf{L}}_{\mathbf{Q}}^\dagger \tilde{\mathbf{L}}_{\mathbf{Q}} \rho \right\} \quad (99)$$

⁴ In the same limit $m/M \rightarrow 0$ the energy shift operator \mathbf{H}_n from (83) turns into a constant, so that it has no observable consequences for a constant gas density.

The corresponding jump operators

$$\tilde{\mathbf{L}}_{\mathbf{Q}} = e^{i\mathbf{x}\cdot\mathbf{Q}/\hbar} \left[\frac{n_{\text{gas}}}{m_*^2} S(\mathbf{Q}, \mathbf{P}) \sigma_B(\mathbf{Q}) \right]^{1/2}, \quad (100)$$

are determined by the cross section in Born approximation, $\sigma_B(\mathbf{Q}) = |f_B(\mathbf{Q})|^2 = |f_B(-\mathbf{Q})|^2$, rather than the individual scattering amplitudes. As a result, the momentum operator \mathbf{P} shows up with a particularly simple functional dependence, given by the dynamic structure factor (98). Recently, the behavior of this equation was studied by means of a Monte Carlo simulation [38].

The weak coupling form of the QLBE coincides with the expression derived earlier by one of us in Ref. [12] (as can be seen if one combines the Eqs. (2) and (25) of that article, setting $\tilde{t}(\mathbf{q}) = -f_B(\mathbf{q})/4\pi^2\hbar m_*$ and $z = n\lambda_{\text{th}}^3$). This agreement is quite remarkable, given the very different type of argumentation in [12], and it serves to corroborate the validity of the present result.

Incidentally, Eq. (99) also shows that the full QLBE *cannot* be obtained from the weak-coupling result by simply replacing f_B by the proper scattering amplitude. This procedure would be ambiguous since the exact scattering amplitude is not just a function of the momentum transfer. As discussed at the end of Sect. V, the dependence of the scattering amplitudes on the tracer particle momentum, which dropped out in the Born approximation, is required if one wants to cover the full set of pairs of scattering trajectories allowed under energy and momentum conservation.

In this context, it is worth mentioning that similar equations are obtained from a heuristic method of dealing with products of delta functions like the ones encountered in Sec. IV B, see e.g. [8, 39]. There, one of the energy delta functions is replaced by a finite Fourier integration over the ‘elapsed time’ as is done in derivations of Fermi’s golden rule. Effectively, this amounts to a treatment in second order perturbation theory where it is permissible to identify the interaction Hamiltonian with the Born approximation of the T-matrix. Although this brings scattering theory language into the game, one should not be tempted to conclude that the non-perturbative equation can be obtained by using the exact T-matrix.

E. Index of refraction

An application of the QLBE involving a rather special limit concerns the interference of matter waves in a Mach-Zehnder setup, where two interference paths are spatially separated by a macroscopic distance. One may ask how the interference fringe pattern changes if the particle is allowed to interact with a background gas in one of the interferometer arms. This setup was realized experimentally with Na and Li atoms [27, 28, 31] (and it is a common configuration in neutron interferometry where the “background gas” consists rather of thermalized condensed matter [40, 41]).

In these situations the beam is strongly collimated, while the likelihood of double collisions is small, so that after any collision that changes the momentum of the interfering tracer particle the latter will be blocked by the interferometer apertures. As a consequence, only forward-scattered amplitudes may contribute to the interference pattern, thus making the energy shift (30) directly observable as a change in the phase of the interference pattern. At the same time an attenuation of the recorded signal is observed.

The phase shift is usually accounted for by attributing a real index of refraction n_1 to the gas, which describes the modification of the de Broglie wavelength due to the energy shift. Exploiting the analogy between the force-free Schrödinger equation and the Helmholtz wave equation [40, 42] the index of refraction for matter waves is determined by the ratio of the energy shift $E_n(\mathbf{P})$ from (30) to the vacuum kinetic energy $E_{\text{kin}} = P^2/2M$ of the particle,

$$\begin{aligned} n_1^2 &= 1 - \frac{E_n(\mathbf{P})}{E_{\text{kin}}(\mathbf{P})} \\ &= 1 + 4\pi\hbar^2 \frac{n_{\text{gas}}}{P^2} \frac{M}{m_*} \int d\mathbf{p}_0 \mu(\mathbf{p}_0) \\ &\quad \times \text{Re} \left[f \left(0; \frac{1}{2m_*} [\text{rel}(\mathbf{p}_0, \mathbf{P})]^2 \right) \right]. \end{aligned} \quad (101)$$

Here we took a rotationally invariant scattering amplitude, $f(\mathbf{p}_f, \mathbf{p}_i) = f(\theta; E_{\text{rel}})$, with $\theta = \angle(\mathbf{p}_f, \mathbf{p}_i)$ and $E_{\text{rel}} = p_i^2/2m_*$.

The index of refraction is typically close to unity, and therefore well approximated by the linearization

$$n_1 = 1 + 2\pi \frac{n_{\text{gas}}}{K^2} \frac{M}{m_*} \text{Re}\langle f \rangle, \quad (102)$$

where $K = P/\hbar$ is the wavenumber of the interfering particle and $\text{Re}\langle f \rangle$ denotes the real part of the thermally averaged forward scattering amplitude,

$$\langle f \rangle = \int d\mathbf{p}_0 \mu(\mathbf{p}_0) f \left(0; \frac{1}{2m_*} [\text{rel}(\mathbf{p}_0, \mathbf{P})]^2 \right). \quad (103)$$

It is common in optics to account for the absorption in a medium by introducing an imaginary part to the index of refraction, which describes the exponential decay of the beam intensity. In the case of a background gas the tracer particles do not get absorbed, of course. However, for a strongly collimated particle beam one expects an exponential decay of the beam intensity after a distance L , since collisions with the background gas decrease the probability of remaining in the beam, thus reducing the fraction of particles taking part in the coherent, wave-like behavior. The decay may be described by neglecting the gain term in Eq. (85), and integrating the remaining equation $\partial_t^{\text{coll}} f_{\text{p}}(\mathbf{P}) = -M_{\text{out}}^{\text{cl}}(\mathbf{P}) f_{\text{p}}(\mathbf{P})$ up to time $t = L/V$, with $V = P/M$, yields the reduction factor $\exp(-M_{\text{cl}}^{\text{out}}(\mathbf{P}) L/V)$. By comparing this to the damped

intensity of a wave, $\exp(-2n_2KL)$, one finds

$$n_2 = \frac{M_{\text{cl}}^{\text{out}}(\hbar K)}{2\hbar K^2/M}. \quad (104)$$

Inserting $M_{\text{cl}}^{\text{out}}$ from (21) and using the optical theorem [20], that is, $p_i\sigma_{\text{tot}}(\mathbf{p}_i) = 4\pi\hbar \text{Im}[f(\mathbf{p}_i, \mathbf{p}_i)]$, one gets an expression analogous to (102),

$$n_2 = 2\pi \frac{n_{\text{gas}}}{K^2} \frac{M}{m_*} \text{Im}\langle f \rangle, \quad (105)$$

with $\text{Im}\langle f \rangle$ the imaginary part of (103). It follows that the combined effect of the energy shift and the reduction of the amplitude of the coherent beam can be described by a complex index of refraction $n = n_1 + in_2 = 2\pi n_{\text{gas}}M/(m_*K^2)\langle f \rangle$.

In case of a Maxwell-Boltzmann distribution (94) the average takes the form

$$\begin{aligned} \langle f \rangle &= \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{dv}{v_\beta} \frac{v}{V} \sinh\left(\frac{2vV}{v_\beta^2}\right) \exp\left(-\frac{v^2 + V^2}{v_\beta^2}\right) \\ &\quad \times f\left(0; \frac{m_*}{2}v^2\right), \end{aligned} \quad (106)$$

with $V = \hbar K/M$ the velocity of the interfering particle and $v_\beta = p_\beta/m$. This expression of the thermally averaged forward scattering amplitude coincides with the one obtained by C. Champenois and collaborators in Ref. [43, 44] with a very different argumentation. It is used in the analysis of the recent experiment with Li atoms [31]. We note that the earlier experiments [27, 28] and the corresponding theoretical treatments [29, 30] were based on different expressions for $\langle f \rangle$ which we consider incorrect, see also the discussion in [44].

F. Diffusive limit

A final important border case is the diffusive limit which is applicable if the tracer state is close to thermal and if its mass is much greater than the gas particle mass, so that the motion is characterized by small momentum transfers. As discussed in [45], an expansion of the jump operators (80) to second order in the tracer position and momentum operators \mathbf{X} and \mathbf{P} is then permissible. In the special case of a *constant* scattering cross-section $|f(\mathbf{p}_f, \mathbf{p}_i)|^2 = \sigma_{\text{tot}}^{\text{const}}/4\pi$ the QLBE then transforms into the generalized Caldeira-Leggett master equation

$$\begin{aligned} \tilde{\mathcal{L}}\rho &= -\frac{i}{\hbar} \frac{\eta}{2} \sum_{i=1}^3 [\mathbf{X}_i, \{\mathbf{P}_i, \rho\}] - \frac{D_{pp}}{\hbar^2} \sum_{i=1}^3 [\mathbf{X}_i, [\mathbf{X}_i, \rho]] \\ &\quad - \frac{D_{xx}}{\hbar^2} \sum_{i=1}^3 [\mathbf{P}_i, [\mathbf{P}_i, \rho]]. \end{aligned} \quad (107)$$

It differs from the original equation [14] in the presence of the last term on the r.h.s of (107), which is necessary to

ensure the complete positivity of the dynamics generated by $\tilde{\mathcal{L}}$ [46]. We emphasize that, unlike in derivations using phenomenological choices for the model environment [47, 48, 49, 50], the friction and diffusion coefficients η and D_{pp} are here uniquely specified by physically measurable properties of the gas. Specifically, the calculation in [45] shows that the friction coefficient η is determined by the temperature, the mass, and the density of the gas, as well as by the scattering cross section,

$$\eta = \frac{8}{3\pi^{1/2}} \frac{n_{\text{gas}} p_\beta \sigma_{\text{tot}}^{\text{const}}}{M}. \quad (108)$$

The momentum diffusion constant D_{pp} is related to η by the fluctuation-dissipation relation

$$D_{pp} = \frac{\eta M}{\beta}. \quad (109)$$

Moreover, the coefficient of the “position-diffusion” term D_{xx} , is already determined by η and D_{pp} , and it is given by the smallest value compatible with complete positivity⁵ [46],

$$D_{xx} = \eta \frac{\hbar^2 \beta}{16M} = \left(\frac{\hbar \beta}{4M}\right)^2 D_{pp}. \quad (110)$$

This shows that the diffusive limit turns the QLBE into the closest possible quantum analogue to the corresponding classical Kramers equation [51].

X. CONCLUSIONS

As seen in the previous section, all relevant limiting cases of the QLBE lead naturally to established master equations. In conjunction with the detailed derivations presented in Sects. IV–VII, this provides ample evidence that Eq. (84) is the appropriate full quantum analogue of the classical linear Boltzmann equation. As such, it serves to describe non-perturbatively and in a unified framework the effects of decoherence and dissipation on a tracer particle.

One reason that seems to have prevented this equation from being formulated earlier is the curious appearance of a second momentum integral in (81) which, in addition to the integration over the momentum exchange \mathbf{Q} , runs over the plane perpendicular to \mathbf{Q} . This makes the equation a bit cumbersome at first sight, at least if represented in a specific basis. However, we have seen in the course of the derivation that this five-dimensional integration is necessary if one wants to cover all the pairs of scattering trajectories which are allowed by both the

⁵ Diósi’s equation [8] leads to the same structure (107), but the “position diffusion” constant D_{xx} is a complicated function of the cross section instead of being simply related to D_{pp} and β .

energy and momentum conservation and by the choice of Q . From a quantum mechanical point of view it is indeed natural to expect that the full set of possible scattering amplitudes contributes to the dynamics. The somewhat unwieldy explicit form is then the inevitable result of the transformation from the center of mass frame, where the scattering transformation takes place, to the laboratory frame needed for the tracer particle coordinate.

Needless to say, the QLBE has a number of limitations. Like the classical linear Boltzmann equation, it cannot be applied in environments where the central Markov assumption is inappropriate, such as liquids. Moreover, it is not applicable at temperatures where the gas is quantum degenerate, and it is far from obvious how this possibility could be incorporated in the framework of the monitoring

approach. Finally, let us reiterate that we presented here a physical derivation which, though stringent and leading to a uniquely distinguished equation, may be hard to substantiate from a formal point of view. An alternative, mathematically more rigorous derivation would be certainly desirable.

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